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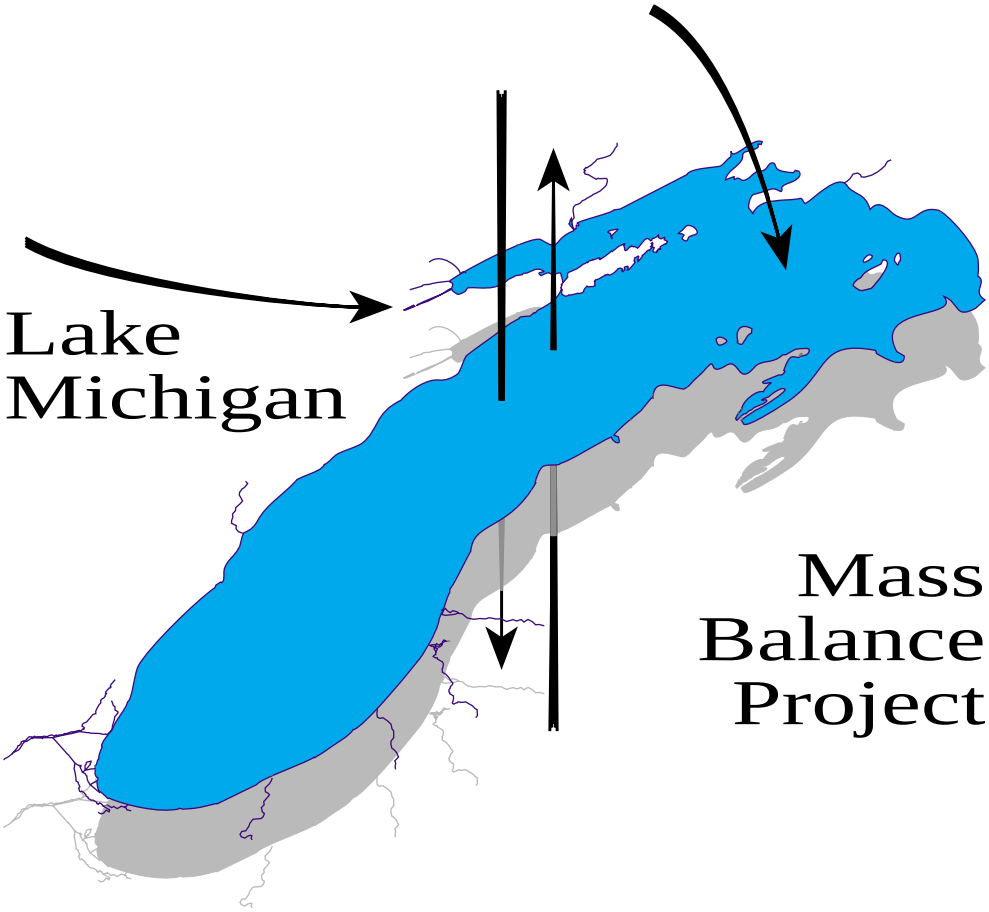
Quality Assurance Plan for Mathematical Modeling



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USEPA-ORD
NHEERL-MED-Duluth
Community-Based Scientific Support Staff
Large Lakes Research Station
Grosse Ile, Michigan 48138

The Lake Michigan Mass Balance Project

Quality Assurance Plan for Mathematical Modeling

by

The Modeling Workgroup

Edited by

William L. Richardson
Douglas D. Endicott
Russell G. Kreis, Jr.
Kenneth R. Rygwelski
Community-Based Science Support Staff
Large Lakes Research Station
Grosse Ile, Michigan 48138

U.S. Environmental Protection Agency
Office of Research and Development
National Health and Environmental Effects Research Laboratory
Mid-Continent Ecology Division--Duluth
Duluth, Minnesota 55804

Notice

The information in this document has been obtained primarily through funding by the U.S. Environmental Protection Agency (USEPA) under the auspices of the Office of Research and Development (ORD) and by the Great Lakes National Program Office (GLNPO). The report has been subjected to the Agency's peer and administrative review and it has been approved for publication as a USEPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Foreword

The Lake Michigan Mass Balance Project (LMMBP) was initiated by the U.S. Environmental Protection Agency (USEPA), Great Lakes National Program Office (GLNPO) to determine strategies for managing and remediating toxic chemicals in the lake basin. Within the ecosystem approach, the mass balance framework is considered the best means of accomplishing this objective and GLNPO requested the assistance of the Office of Research and Development (ORD) in producing mathematical models that account for the input, fate, and food chain bioaccumulation of certain chemicals in the lake. This approach has been used in the past to develop target loads for phosphorus in controlling eutrophication. During an intensive study of Green Bay, it proved to be a reliable and effective means of providing a basic scientific understanding of the ecosystem, mass fluxes, and chemical and biological processes. The approach also proved to be an efficient means of organizing the project and aiding decision-makers in choosing among alternative management options. By focusing federal, state, local and academic efforts and resources on a common goal, much more was accomplished than if these entities acted independently.

This approach requires all monitoring and field research be coordinated and common methodologies used. The product will then be a consistent and reliable database of information that will be accessible by project participants and the public. Data for the LMMBP were collected during 1994 and 1995 and are now being compiled according to specified quality assurance/quality control (QA/QC) requirements.

The means to synthesize and interpret this information needs similar scrutiny. This quality assurance project plan (QAPP) for mathematical modeling provides the basic procedures that all aspects of model development and application will follow. It attempts to follow guidance provided by the USEPA and other agencies in assuring that the scientific theory is implemented accurately and completely by model computer code. It requires modelers to specify the theory and processes included in the models and requires that they document their work.

This QAPP also provides for a scientific review process using an interdisciplinary panel of scientists and experts that will review model theory and application on a continuing basis. The purpose is to ensure that decisions based on the modeling efforts are reliable and scientifically credible.

This plan is not intended to include all of the details and background required to understand the entire LMMBP. Rather the reader should refer to the LMMBP Workplan (USEPA, 1997a) and the Modeling Workplan (USEPA, 1995a, and other documents cited herein). The Modeling Workplan is included as an appendix to this report. Also, readers can access project information via the GLNPO WEB page, http://www.epa.gov/glnpo/lmmb/.

Abstract

This report documents the quality assurance process for the development and application of Lake Michigan Mass Balance models. The scope includes the overall modeling framework as well as the specific submodels that are linked to form a comprehensive synthesis of physical, chemical, and biological processes of Lake Michigan..

The models cited in this report include hydrodynamic, sediment transport, eutrophication, transport chemical fate, and food chain bioaccumulation. In addition, the report includes the quality assurance (QA) process for the development of atmospheric models used to describe the emission of atrazine from the agricultural portion of the watershed and its transport and deposition to the lake. It also includes the QA process for the estimation of tributary and atmospheric loads for atrazine, polychlorinated biphenyls (PCBs), *trans*-nonachlor (TNC), and mercury.

This report does not include the QA process for field collection and laboratory analyses. These are covered in separate documents (USEPA, 1997b,c,d,e).

With the ever increasing costs of environmental regulation and remediation, the reliance on scientific interpretation of information, and the need to forecast future impacts, USEPA is placing more emphasis on the quality and credibility of the synthesis process and tools. The Agency has issued several documents covering broad requirements of the development and use of mathematical models and these are used in the formulation of the plan for Lake Michigan. Because this guidance is new and somewhat limited, this QAPP is a prototype for this process which includes a suite of linked, multi-media models which together form an ecosystem approach.

In the final analysis, the quality of the work and the reliability and credibility of the models will be determined not only by the issuance of a QA plan, but by the desire and integrity of the project personnel. History has shown the mathematical models of Great Lakes water quality to be reliable in predicting future events and determining regulatory and remedial strategies that have been successful. The Lake Michigan modeling efforts build on this long history of model development by the ORD's Great Lakes Modeling Program at Grosse Ile, Michigan, the Modeling Program at Research Triangle Park, North Carolina, the experience of the National Oceanic and Atmospheric Administration (NOAA) Great Lakes hydrodynamic modeling program at the Great Lakes Environmental Research Laboratory (GLERL) in Ann Arbor, Michigan, and the Modeling Program of the U.S. Army Corps of Engineers (USACOE) at Waterways Experiment Station (WES), Vicksburg, Mississippi. In addition, it relies upon the experience and knowledge of other federal, private, and academic organizations.

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Acronyms and Abbreviations

AMD	Atmospheric Modeling Division
AQSM	Air quality simulation models
AREAL	Atmospheric Research and Exposure Assessment Laboratory
CAAA-90	Clean Air Act Amendments of 1990
CBSSS	Community-Based Science Support Staff
CEAM	Center for Exposure and Assessment Modeling
CGEIC	Canadian Global Emissions Interpretation Centre
CILER	Cooperative Institute for Limnology and Ecosystem Research
CTF	Contaminant transport and fate model
CWA	Clean Water Act
DOC	Dissolved organic carbon
EMP	Enhanced Monitoring Program
ESD	Eutrophication sorbent dynamics model
GBMBS	Green Bay Mass Balance Study
GLERL	Great Lakes Environmental Research Laboratory
GLNPO	Great Lakes National Program Office
GLWQA	Great Lakes Water Quality Agreement
Hg	Mercury
HOC	Hydrophobic organic chemicals
IJC	International Joint Commission
LaMPs	Lake-wide Management Plans
LLRS	Large Lakes Research Station
LMMBP	Lake Michigan Mass Balance Project
MED-Duluth	Mid-Continent Ecology Division-Duluth
MM5	Mesoscale Meteorological Model
NCAR	National Center for Atmospheric Research
NERL	National Exposure Research Laboratory
NHEERL	National Health and Environmental Effects Research Laboratory
NOAA	National Oceanic and Atmospheric Administration
NWS	National Weather Service
ORD	Office of Research and Development
PCB	Polychlorinated biphenyls
POC	Particulate organic carbon
POM	Princeton Ocean Model
PSU	Penn State University
QA	Quality assurance
QAPP	Quality assurance project plan
QC	Quality control
QSIP	Quality systems and implementation plan

RADM	Regional Acid Deposition Model
RAPs	Remedian Action Plans
RCS	Revision Control System
RDMQ	Research Data Management and Quality Control System
RPM	Regional Particulate Model
SUNY	State University of New York
TNC	*trans*-nonachlor
UCSB	University of California-Santa Barbara
UMAQL	University of Michigan Air Quality Laboratory
USACOE	United States Army Corps of Engineers
USCG	United States Coast Guard
USDA	United States Department of Agriculture
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
WASP	Water Quality Simulation Program
WDNR	Wisconsin Department of Natural Resources
WES	Waterways Experiment Station

Acknowledgments

This report has been prepared by the members of the Lake Michigan Mass Balance Project, Modeling Workgroup and with review and comments by many other persons too numerous to list here. However, the primary impetus to complete this plan originated with Paul Horvatin, GLNPO, who has paid diligent attention to the QA aspects of the entire project. Louis Blume, GLNPO, and Al Batterman, Mid-Continental Ecology Division-Duluth (MED-Duluth), provided review from an overall QA perspective. Linda Kirkland also provided essential comments on the preliminary draft. The editors appreciate the talents of Debra Caudill for her diligent and skillful job in formatting the final document and of Kay Morrison and her artistic abilities in preparing the figures.

Chapter 1
Introduction

A primary component of the Lake Michigan Mass Balance Project (LMMBP) involves the development and application of mathematical models relating the sources of chemicals to their concentration in air, water, sediment, and biota. Models integrate the complex transport and fate processes involved in determining mass balances of important chemicals and predicting future conditions under a variety of alternative management scenarios. Because of the economic and environmental consequences of pending decisions, care must be taken to ensure the quality, dependability, accuracy, and scientific credibility of all aspects of the project. This quality assurance (QA) plan for the modeling aspects of the project will help ensure that these goals are achieved.

The Modeling Workgroup members prepared this plan under the direction of the Chairperson, William L. Richardson, P.E., Environmental Engineer, U.S. Environmental Protection Agency (USEPA), Office of Research and Development (ORD), National Health and Environmental Effects Research Laboratory (NHEERL), Mid-Continent Ecology Division-Duluth (MED-Duluth), Community-Based Science Support Staff (CBSSS), Large Lakes Research Station (LLRS), Grosse Ile, Michigan. Guidance for the preparation of the plan has been obtained from several sources including:

> Quality Assurance Guidelines for Modeling Development and Application Projects: A Policy Statement. Environmental Protection Agency, ERL-Duluth. November 1991.
>
> Reducing Uncertainty in Mass Balance Models of Toxics in the Great Lakes--Lake Ontario Case Study. Great Lakes Program, State University of New York at Buffalo. February 1993.
>
> Agency Guidance for Conducting External Peer Review of Environmental Regulatory Modeling. Agency Task Force on Environmental Regulatory Modeling. July 15, 1994.
>
> National Exposure Research Laboratory Position Paper on Multimedia Modeling, Third Draft. USEPA, NERL. May 19, 1995.
>
> Standard Practice for Evaluating Mathematical Models for the Environmental Fate of Chemicals. ASTM, Designation: E 978-92.

Background

The LMMBP was initiated by the USEPA Great Lakes National Program Office (GLNPO) cooperation with the USEPA/ORD and other federal and state agencies. The project was initiated in response to regulatory mandates contained in the Great Lakes Water Quality Agreement (GLWQA) between the United States and Canada and federal legislation that requires the development of "Remedial Action Plans" (RAPs) and "Lake-wide Management Plans" (LaMPs). The purpose is to restore and maintain the chemical, physical, and biological integrity of the waters of the Great Lakes Basin ecosystem. USEPA also intends that the LaMP process serves as the basis for the development of State Water Quality Management Plans. This project also has implications and applications to the Great Lakes Binational Toxics Strategy (Virtual Elimination Strategy) and the Great Waters Program.

The primary goal of the LaMP is to develop a sound scientific base of information to guide future toxic load reduction efforts at the federal, state, tribal, and local levels. Objectives include: (1) identification of relative loading rates of critical pollutants from major sources to the Lake Michigan Basin; (2) to evaluate relative loading rates by media (tributaries, atmospheric deposition,

contaminated sediments) to establish a baseline loading estimate to gauge future progress and load reductions; (3) develop the predictive ability to determine the environmental benefits of specific load reduction scenarios and the time to realize those benefits; and (4) improve our understanding of key environmental processes which govern the cycling, dynamics, and availability of contaminants within relatively closed ecosystems. These objectives are consistent with those of the LMMBP and with the need for multi-media mathematical modeling in an ecosystem approach. The primary pollutants of concern are polychlorinated biphenyls (PCBs), *trans*-nonachlor (TNC), atrazine, and mercury. These contaminants have different sources, environmental behaviors, modes of action, and pose different threats to the ecosystem's food web as well as wetlands, wildlife and fisheries. The target species for this investigation are lake trout and coho salmon; however, the supporting food chains of each of the primary species require examination.

In addition, the project was to be synchronized with the States' "Enhanced Monitoring Program." A series of preliminary meetings was held to discuss the need and organization of the project. A committee structure was developed and implemented. Under the direction of a Steering Committee and Technical Coordinating Committee, a detailed workplan was prepared (USEPA, 1997a). The Modeling Workgroup prepared a Modeling Workplan (USEPA, 1995a) which guided the project design. A Program QA Plan (USEPA, 1997b) was prepared for the project but did not directly include QA for mathematical modeling. Subsequent QA audits of the project determined the need for a specific modeling QA plan.

In addition to the project workplan, modeling workplan and QA plan, a methods compendium (USEPA, 1997c,d,e), data administrative plan (USEPA, 1995b), and data reporting format (USEPA, 1997f) have been prepared (access these documents via the GLNPO web page: http:/www.epa.gov/glnpo/lmmb/). The project planning scheme is shown in Figure 1.

These provide the documentation infrastructure for QA of field, laboratory, data, and database management aspects which support project information being utilized by the models. Because the documents are available elsewhere, these aspects will only be summarized in this report.

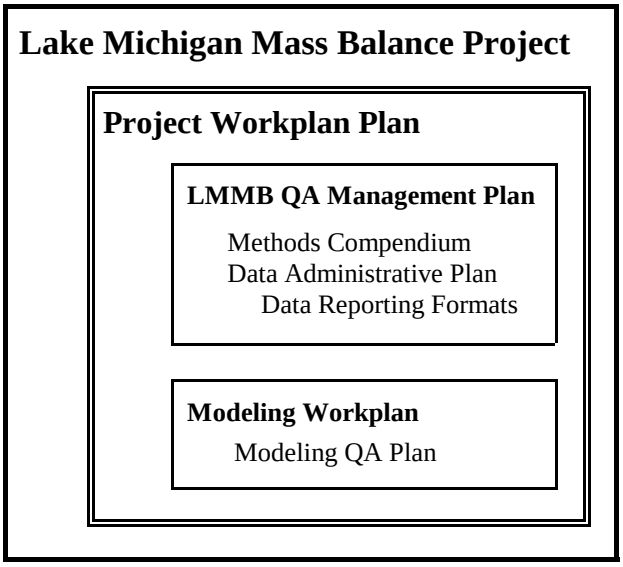

Figure 1. Lake Michigan Mass Balance Project Workplan Diagram.

General Considerations for Modeling Quality Assurance

Traditionally, scientific and engineering philosophy and ethics profess a high regard for QA and quality control (QC). Within USEPA and ORD, quality of science has been a primary and over-riding consideration in project planning and execution. But within the regulatory context of USEPA, meeting deadlines is also important and there are always judgements made on the trade-offs between quality (primarily in terms of thoroughness and complexity) and timeliness. When quality is sacrificed in lieu of timeliness, there may be severe consequences. The space shuttle Challenger disaster exemplifies this well. The approach for this plan attempts to attain a balance without sacrificing scientific credibility, accuracy, and thoroughness. The challenge is to assemble the necessary scientific/modeling experts, to determine the best mix of modeling theory and approaches, to use the most current modeling computer programs, and to modify and apply these to the scientific and management issues confronting Lake Michigan. This must be done with resource constraints and with a common sense approach to meeting project timeliness.

There are limitations with the level or detail of modeling that can be accomplished within the budgets available. For example, it would be desirable and preferable to

develop and apply a three-dimensional model of sediment transport. This was the original intent but, because of budgetary constraints and personnel limitations, this was changed and a compromise was made to use an existing two-dimensional model to help understand sediment transport processes. Although this is not perfect, it will reflect state-of-the-art modeling for the Great Lakes. Credibility will be achieved by carefully qualifying model results, defining the uncertainty of the calculations, and ensuring that the models are correct within the appropriate time and space scales.

It should be understood that the modeling efforts for this project build upon a rich history of Great Lakes research conducted by the USEPA and its partners. This history adds considerable credibility to the Lake Michigan modeling endeavors. Much of this history has led to the approaches that are being used to ensure quality for the present project. These include the following factors:

1. Qualified personnel including education, training, experience, expertise, integrity, and publication record.

2. Infrastructure including laboratories and offices, computers, software tools, supporting administrative staff and progressive and supportive management.

3. Adequate extramural research budgets for acquisition of expertise beyond that of the in-house research staff.

4. The administrative means to include extramural researchers and contractors via cooperative agreements and contracts including the ability to build coordinated teams and partnerships directed at answering relevant scientific and management questions.

5. Interaction within the scientific and engineering communities at scientific meetings and workshops and through publications in journals to ensure the utility of most currently accepted scientific theory.

6. Professional engineering judgement.

7. Computer programming support to implement the theory into computer code.

8. Verification of computer code and calculations.

9. Evaluating and reporting uncertainties of calculations and stating assumptions, qualifications, and caveats which could affect research application to regulatory problem-solving.

10. Peer review of research including theoretical construct, computational methodology, appropriateness of application, assumptions, and interpretations.

11. Common sense and hard work.

These factors are incorporated into this QA Plan for Lake Michigan.

Basis of Great Lakes Modeling Quality Assurance

The Lake Michigan models build on over two decades of modeling research, conducted by USEPA, ORD, and its cooperators. In 1971, the International Field Year on the Great Lakes was initiated as an interagency endeavor to investigate the physical, chemical, and biological status of Lake Ontario. The first calibrated, eutrophication model for a Great Lake resulted (Thomann and Di Toro, 1975). A series of projects was conducted by the ORD Great Lakes Modeling Program at the Grosse Ile Facility (LLRS) from 1973 through about 1980 in response to the research requirements of the U.S. Canada GLWQA with direction from the International Joint Commission (IJC). Field studies were conducted on Lake Erie, Lake Huron, and Lake Michigan that provided baseline observations and input information to construct eutrophication models for each of those lakes and for Saginaw Bay (Bierman and Richardson, 1976; Richardson, 1976; Di Toro and Matystik, 1980; Rodgers and Salisbury, 1981; Bierman *et al*., 1984; Bierman and McIlroy, 1986; Bierman and Dolan, 1986).

In 1977 toxic chemicals became a primary concern for the Great Lakes. USEPA/ORD responded with the development of the first PCB models for the Great Lakes (Richardson, *et al.*, 1983; and Connolly, 1984; Thomann and Di Toro, 1984). Related to the special needs of the Great Lakes, ORD developed the capability of analyzing PCB congeners at ultra trace levels.

These experimental and modeling endeavors were carried out by teams of investigators under the direction of USEPA principal investigators and project officers. Much of the pioneering modeling research was done by a group of environmental engineers at Manhattan College, Riverdale, New York. Expertise grew over the past 25 years and as a result, a Great Lakes "modeling community" emerged including scientists and engineers from a number of universities, government research laboratories, and private consulting firms.

The Great Lakes modeling community's efforts included fate and bioaccumulation modeling of PCBs and other toxic chemicals for the Great Lakes (Thomann and Connolly, 1984), modeling of toxicity for the Raisin River and Detroit River (Di Toro *et al*., 1985a,b, 1986, 1988), screening level modeling for PCBs, tetrachlorodibenzo-p-dioxin (TCDD), atrazine, and other chemicals for Lake Michigan, Green Bay, and Lake Ontario (Martin *et al*., 1989; Endicott *et al*., 1991, 1992).

These efforts culminated in the development and application of toxic chemical models for the lower Fox River and Green Bay. During this study, GLNPO requested ORD to lead the modeling efforts. The field and laboratory efforts were designed according to the modeling requirements. This project could be viewed as the definitive Great Lakes modeling effort to date (Connolly *et al*., 1992; Bierman *et al*., 1992; DePinto *et al*., 1993; HydroQual, 1995; Martin *et al*., 1995; Lick *et al*., 1995; Velleux *et al*., 1995, 1996; Richardson *et al*., 1997). This effort demonstrated the feasibility of the mass balance modeling approach in a large embayment. QA for modeling was not a formal requirement within this study; however, an on-going peer review process whereby modelers presented their research plans, interim results and final results at meetings, workshops, and scientific conferences during the entire project provided more than sufficient scrutiny to assure a credible product in the end.

Several approaches can be taken to examine model credibility including calibration to observed data, verification of predicted or historical conditions over time, and paleolimnological methods. Another approach includes checking the validity of different models in response to the same problem. This has been part of the history of Great Lakes modeling research. For example, in the development of target loads for phosphorus under the GLWQA, a number of models were developed and applied for Lake Erie at various levels of spatial and chemical resolution. Comparison of model predictions provided at least one test of model credibility (Di Toro *et al*., 1987; Bierman and Dolan, 1986).

Another case involved the development and application of a model for toxic chemicals including dioxin in Lake Ontario. Insufficient data were available for model calibration so two models were used to gain credibility. These models had been developed independently by two modeling groups, unique theoretical constructs, and different computer programs and solution techniques. The final predictions of chemical concentration made by these different models were nonetheless comparable. During this project, the model computer programs and input data sets were provided to an independent review panel. This panel reviewed the model constructs, input data sets, and re-ran the models to reproduce results before submitting their assessments.

In a limited number of cases, models developed over 20 years ago have been post-audited and serve as a form of model verification and validation (Di Toro and Connolly, 1980; Di Toro *et al*., 1987; Zahakos *et al*., 1993; Chapra and Sonzogni, 1979; Lesht *et al*., 1991; Bierman and Dolan, 1986; Bierman *et al*., 1984). Annual loading estimates over the validation period were used in the models to simulate concentrations over the same time period. Although results vary somewhat, good agreement between model predictions and field data are generally observed. The agreement between predicted and observed concentrations indicate the predictive capabilities of the models and their known certainty.

Until recently, formal QA plans were not required for Great Lakes model development or application. Even so, the model theory and computer programs developed have been used successfully throughout the world for investigations of many important pathways. So lack of a QA plan and auditing process does not imply models are less credible nor does the inclusion of a QA plan necessarily ensure that models are correct. In the final analysis, model credibility depends on many factors and a QA plan will help ensure these factors are taken into consideration in a formal, logical manner.

Preparation of this QA plan has required considerable effort but in the long run should save time by reducing errors, minimizing corrections and reanalysis, and

reducing the need for continual explanations and justifications. The process also allows the modelers to present their views concerning resources required and to clarify expectations.

Much of the background work was done before the formal QA document was begun. A Modeling Workplan (USEPA, 1995a) was developed by the modeling staff at Grosse Ile and the modeling workgroup including staff from the National Exposure Research Laboratory (NERL) in Research Triangle Park, North Carolina. This plan, which included specification of the Lake Michigan Enhanced Monitoring Program, was submitted to the Technical Coordination Committee for use in developing the overall project workplan. Although a formal QA plan had not been in place by the commencement of the project, considerable work had been done that logically belongs to this plan.

Background of Air Quality Modeling

When concern over air quality developed in the United States and Canada several decades ago, the problem appeared to consist essentially of excessive local concentrations of common pollutants such as sulfur dioxide, particulates, carbon monoxide, and ozone. Air quality is now recognized as a much more complex problem or group of problems that span many pollutants having media-specific behaviors over very large geographic areas.

The role of atmospheric transport and deposition to the Great Lakes basin has been addressed under several modeling constructs, including mass balance models. In principle, the complex movements of pollutants through different parts of the environment can be described through a mass-balanced model. In practice, however, the data requirements needed to make reasonable estimates of the many processes involved are large, and sufficient data for these calculations usually are not available. Uncertainties are substantial even with the best available data on atmospheric and non-atmospheric inputs. The LMMBP will seek to reduce uncertainty in the atmospheric component of the mass balance by employing mathematical models of atmospheric transport and deposition, to provide estimates for spatial and temporal gaps in actual monitoring databases, and to test hypotheses about characterizations of atmospheric transformations and removal.

Air Quality Simulation Models (AQSMs) are frequently used to characterize the emission, transport, and deposition of hazardous air pollutants over large geographic areas. These models incorporate fairly extensive source emission inventories and meteorological databases (e.g., wind fields, temperature, mixing height) and apply the collected data to simulated processes such as dispersion, transformation, and deposition. The models are run to generate estimates of pollutant concentrations and deposition rates over a spatial and temporal pattern.

The mathematical relationships between emissions and concentration (or deposition) are typically nonlinear, due to the influences of the atmospheric transport, chemical and physical transformation, and deposition processes. Therefore, one cannot extrapolate, based on measurements alone, the quantitative relationship between changes in emissions and changes in atmospheric concentrations (or deposition). AQSMs attempt to account for the nonlinear physical and chemical processes influencing atmospheric concentrations deposition.

Development of AQSMs started in the late 1970's. The Urban Airshed Model (UAM; Scheffe and Morris, 1993) followed by the Regional Oxidant Model (ROM; Lamb, 1983) provided Eulerian-based models for ozone, the former for urban and the latter for regional scale. Strategies for State Implementation Plans (SIPs) used ROM to provide boundary conditions for UAM simulations. Attention to acid deposition issues was addressed in the 1980's with the development and evaluation of regional acid deposition models such as the Regional Acid Deposition Model (RADM; Chang *et al*., 1987), the Acid Deposition and Oxidant Model (ADOM; Venkatram *et al*., 1988) and the Sulfur Transport and Emission Model (STEM; Carmichael *et al.*, 1986). Other major modeling systems included the Regional Lagrangian Modeling of Air Pollution model (RELMAP; Eder *et al*., 1986), a Lagrangian framework system, and semi-empirical and statistical models. Models of this period were designed to address specific air pollution issues, such as ozone or acid deposition. Thus, flexibility to deal with other issues such as particulate matter or toxics was very limited. With the passage of the Clean Air Act Amendments of 1990 (CAAA-90), a wide range of additional issues was identified including visibility, and fine- and coarse-particles, as well as indirect exposure to toxic pollutants such as heavy metals, semi-volatile organic species, and nutrient deposition to water bodies.

In the 1990's, the USEPA embarked upon the development of an advanced modeling framework to meet the challenges posed by the CAAA-90. The Models-3 framework has been designed for holistic environmental modeling utilizing state-of-science representation of atmospheric processes in a high performance computing environment. Descriptions of Models-3 can be found in Novak *et al*. (1998) and Byun *et al*. (1998). The science components in Models-3 are called the Community Multi-scale Air Quality (CMAQ) system and are described briefly in Ching *et al*. (1998). The Models-3/CMAQ system is designed as a multi-pollutant, multi-scale Eulerian framework air quality and atmospheric deposition modeling system. It contains state-of-science parameterizations of atmospheric processes affecting transport, transformation, and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species. It is the new modeling system that will be further enhanced and applied to address the specific areas of concern for the LMMBP.

Chapter 2
Common Quality Assurance Topics as Applied to All Project Models

Because the LMMBP modeling framework consists of a series of linked models, general QA aspects that apply to all of the models will be presented first. Aspects of each model will then be presented individually in Chapter 3. Also, because many of these models are under development, it is impossible to provide all of the detailed information immediately. Rather, as models are developed, tested, and applied, the information will be updated as future addenda to this report.

The general and specific details that follow are presented in the format suggested by modeling QA guidelines (USEPA, 1991). Some additional sections are included that fulfill more recent Agency requirements.

Modeling Quality Objectives and Acceptance Criteria

Before a model is used for remedial guidance and/or regulatory purposes, there needs to be some agreement between the expectations of the managers who will be using the model and the model developers. Managers need to be versed in the science of modeling natural systems. They should realize that simulating natural phenomena, unlike controlled systems like electrical or mechanical systems, is very difficult because of the inherent variability and ever changing biological structures. Modelers have the responsibility of not only attempting to make the models reliable, but to state unequivocally their assumptions and uncertainties. This is usually done by providing the most probable answer(s) along with uncertainty brackets which provide the probability that the actual answer is contained within a range. The decision-maker must determine whether to use the model with the uncertainties and caveats provided, or to provide additional resources to refine the results.

There is an attempt within this document to help managers determine the degree to which the models will be calibrated to field data. This constitutes the project acceptance criteria and reflects what can practically be done with the resources commitments. Basically, the criteria for accepting the modeling results lies in the ability to simulate measured concentrations of materials in water, sediment, and biota during the field collection period. If this is done within the statistical range required, then the model(s) can be used to extrapolate these concentrations in space and time. Model validation is beyond the scope of the project. Validation is defined as the process by which model predictions are compared to measurements made at some future time. This may ultimately be done, but has not been included (by management) as a requirement. Modelers attempt to use whatever data are available and many of the model simulate historical data. This should be viewed as an additional rationale for model acceptance.

The modeling quality objectives are incorporated into the LMMBP's "data quality objectives (DQO)" in the overall QA plan (USEPA, 1997b):

> "After following the DQO process, LMMBP Study managers agreed that the overall LMMBP Study DQO was to develop a model capable of calculating pollutant concentrations in Lake Michigan to within a factor of two of observed concentrations in the water column and target fish species. Study managers also agreed to accept an uncertainty level for each input to the model that is within 20-30% of the mean at the 95% confidence interval."

The DQO was developed by members of the Technical Coordinating Committee and participating government employees. Discussions were held between the QA

managers and government modelers. The QAPP was approved by the Executive Steering Committee. Names and organizations of participating personnel are listed in Appendix F.

This statement is interpreted by the modelers to mean that the project's monitoring, surveillance, and analytical programs were established in an attempt to define all model forcing functions and state variables within 30% of the actual values. The modeling objective is to simulate the average water quality within plus or minus two standard errors of the mean (by cruise/segment average). Plus or minus two standard errors means that there is 95% confidence that the actual mean falls within this range. The range should be within 30% of the mean if sampling and analysis design is correct. This is the goal for all state variables for all segments by cruise or collection group. The data means and standard errors will be computed using statistical interpolation/extrapolation techniques such as found in contouring or kriging algorithms.

In addition, model simulations will attempt to reproduce the statistical distribution properties of the data. This will be evaluated by comparing cumulative frequency distribution plots of data to frequency distribution plots from comparable model predictions.

Prediction bias will be minimized by calibration, the process of parameter optimization seeking to minimize residuals (the difference between calculated and measured concentrations), without violating constraints imposed by scientific observations and principles. Methods of calculating or estimating loadings or other forcing functions may be refined, if necessary, but no calibration of forcing functions will be allowed. The goal for bias reduction is to remove any apparent spatial or temporal trends in residuals. Practically, this means that residuals are uncorrelated and reduced to the magnitude of analytic or replication errors.

The uncertainty of model predictions will be estimated using a two-step procedure. The parameter variance-covariance matrix resulting from calibration will be estimated; then, this matrix will be applied to generate exceedence levels for model predictions using Monte Carlo methods. While it is not possible to make *a priori* estimates of prediction uncertainty, the goal is 95% exceedence limits within a factor of two of the predicted toxic chemical concentrations in water and top predator fish over the duration of the calibrated period (1994-95).

Project Description

Scope, Purpose, Objectives

The project description including scope, purpose, and objectives is provided in the project workplan (USEPA, 1997a), in the modeling workplan (USEPA, 1995a), and are summarized in Chapter 1 of this report. Rather than repeating the details, the Modeling Workplan is included here as Appendix A. It should be noted that the Workplan continues to be revised as the feasibility of various aspects of the project are determined. Another source of general project information can be accessed on the GLNPO Web site: http://www.epa.gov/glnpo/lmmb/.

In summary, the primary purpose of modeling is to provide the scientific basis for understanding the sources, transport, fate, and bioaccumulation of toxic chemicals in Lake Michigan. Once a scientifically sound suite of models are developed, they can be used to forecast future in-lake chemical concentrations under alternative management scenarios. For example, the models will be used to forecast the concentration of PCBs in lake trout. In addition, the models will be capable of discerning the internal and external sources of toxic chemicals in broad categories -- tributary, atmosphere, and sediment.

Specifically, four toxic chemicals are being studied: mercury, PCBs, atrazine, and TNC. The modeling framework includes transport, fate, and bioaccumulation (Figure 2).

The models are being developed and applied at different levels of scale and uncertainty. The first of these has been the development of screening level models. These models attempt to assemble all present knowledge for a given chemical and assess the problem in broad space and time scales. The screening models have been useful in project design by helping define important gaps in knowledge and understanding and directing process research and surveillance efforts to acquire the most useful information to reduce uncertainties. Screening models have been developed for PCBs and atrazine (Endicott *et al*., 1992; Rygwelski *et al.*, 1997). The primary caveat for screening models is that they are not necessarily well-calibrated to field data (or calibrated at all) and that what data exist may

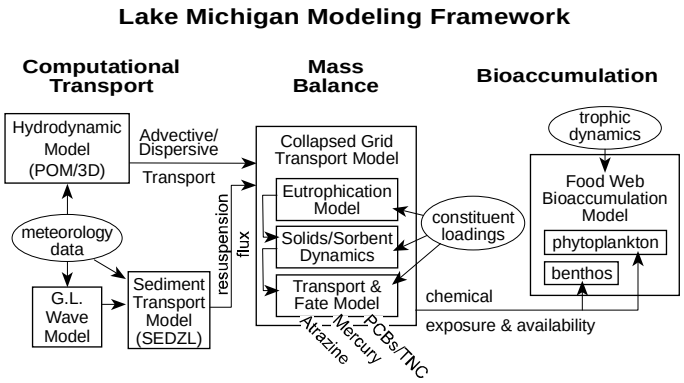

Figure 2. Lake Michigan Modeling Framework.

originate from a variety of sources with inconsistent methodology and quality control. Therefore, these models are not to be used for regulatory decision-making but rather to help in directing research and surveillance efforts, and for, perhaps, providing a basis for scientific and management debate.

The second level of model involves the refinement of the spatial and temporal scales for transport and chemical fate, and biological processes. A medium-resolution segmentation scheme was developed by dividing the lake into 10 horizontal surface segments with five vertical layers and a comparable sediment bed segmentation. At this level of resolution, it will be feasible to calibrate model processes and to begin reliable lake-wide, long-term simulations for management purposes. These level-two models are conceptually similar to screening models except with greater spatial/temporal resolution and with a greater degree of reliability because they are based on calibration using verified field data and loading/forcing function estimates.

At the highest level of resolution, a hydrodynamic model is being applied to simulate the three-dimensional temperature and current structure of the lake. This information, required for water quality modeling, cannot be measured at the necessary spatial and temporal resolution. Hydrodynamic simulations will be performed on a five-kilometer square horizontal grid. A sediment transport model will also be applied at the five kilometer resolution to predict particle transport fluxes due to shoreline erosion, wave-and-current-driven resuspension, and particle settling. Results from both the hydrodynamic and sediment transport models will be used as input to the mass balance models, including eutrophication and contaminant transport and fate.

There are two reasons for pursuing different model levels in the Lake Michigan project. First, modeling at different levels of resolution and process detail yields valuable insight regarding, for example, the trade-off between model complexity and reliability. Modeling is always somewhat experimental, and different "level" approaches will maximize the opportunity for experimentation. This approach has been endorsed by prominent Great Lakes water quality modelers (Mackay and Bierman, 1993) and should lead to a more accurate final modeling product. The second, more practical reason, is that lower-resolution and -complexity models can provide interim results before the higher resolution/complexity models are completed. This is because model programs are available for lower level application, while development continues on the higher level model programs. In addition, development and application proceeds more rapidly using the lower resolution/complexity models, due to factors such as easier input processing, error checking, and calibration, less computational requirements and, lesser user training to gain proficiency.

As mentioned above, all model simulation results will be compared to measurements obtained from the project data collection program. QA in the context of field collection of samples and analytical chemistry, physical, and biological measurements is a very important aspect of this project as well as being a requirement by the Agency. The data requirements for modeling as specified in the Modeling Workplan, Appendix A, have been incorporated into the Project Workplan (USEPA, 1997a) and in the field and laboratory program. A QA plan (USEPA, 1997b) and methods compendium (USEPA, 1997c,d,e) have been prepared and are being implemented for these aspects of the project.

Four primary contaminants were elected for examination in this study: PCBs, TNC, atrazine, and mercury. The Project Workplan (USEPA, 1997a) provides the overall

sample design and media targeted for collection. In summary, these contaminants have been measured in air, tributaries, water, sediment, and biota (atrazine not measured in biota). Nutrients, such as various forms of phosphorus, nitrogen, and silica have also been measured for appropriate media. Additionally, conventional parameters (e.g., chloride, temperature, chlorophyll *a*, organic carbon, etc.) were measured in water samples. Associated studies of sediments, sediment traps, and radiated sediment cores have also been conducted for model calibration procedures.

Target fish species for LMMBP are lake trout and coho salmon. In each case, the supporting food chains of each species also has been examined. Lake trout were collected in south, central, and northern parts of the lake along with forage fish (bloater chub, alewife, smelt, and sculpin). Zooplankton, phytoplankton, and benthic invertebrates were also collected as the lower food. Coho salmon have been collected according to their seasonal migration pattern in the lake. For these samples, the bioaccumulative contaminants have been analyzed. Supporting data such as age, weight, length, percent lipid, percent moisture, etc., have also been collected. Gut content studies on target and forage fish have been conducted to examine seasonal and temporal food web relationships.

In all cases, the partners responsible for collection and analysis have provided workplans, QA plans, and standard operating procedures (SOPs) for each aspect in accordance with the Project Workplan (USEPA, 1997a) and the Project QA Plan (USEPA, 1997b). These have been reviewed and approved by Project QA Management. Additionally, field sampling methodologies are found in USEPA, 1997c, and laboratory analysis procedures are contained within USEPA, 1997d, and USEPA, 1997c. Quality assurance audits and reviews of the resultant data from the LMMBP are discussed later in this document.

Resources limited the number of samples collected and analyses that could be performed so model evaluation will include estimates of uncertainty. Uncertainty is also a function of what is known about the processes governing the transport, fate, and bioaccumulation of each chemical. More is known for PCBs as this chemical has been the subject of intensive research and modeling efforts in the past. Less is known about the other chemicals, particularly mercury. A first attempt will be made to balance mass for the total mercury in water and sediment. Refinements to incorporate more of the mercury species and fate processes, as well as examination of some modeling for bioaccumulation in the food chain, will be made as time permits, but it is expected that the mercury model development and application will extend beyond the time frame of the LMMBP.

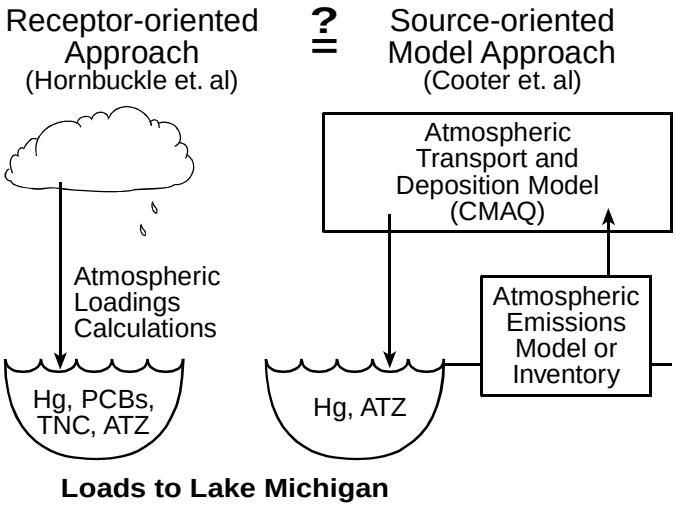

Figure 3. Loads to Lake Michigan

Atmospheric modeling will take two approaches. One will be 'receptor-oriented'; the other will be 'source-oriented'. In the former, estimates of the loads of PCBs, atrazine, TNC, mercury to Lake Michigan will be made by interpolating atmospheric concentration data across the lake. In the 'source-oriented' method, emissions of mercury and atrazine from sources will be estimated and their deposition to the Great Lakes modeled.

Products and Timetable

The products from the modeling efforts will include a final modeling project report including executive summary for each of the contaminants of interest, individual model reports by each modeler or model team, and

documentation of models and other computer programs. In addition, scientific journal publications will be produced. Modeling products will be completed in sequence as project data and loads become available and the modeling process proceeds to an appropriate end point. The preliminary sequence is atrazine, PCBs/TNC, and mercury. Priority will be placed on the management needs of GLNPO and cooperating regulatory agencies and modeling reports will be dovetailed with the overall project reporting schedule which is being determined.

Also, presentations of model results will be made during and after the project. Management presentations will be made at the request of GLNPO and other USEPA and state officials. Scientific presentations will be made at meetings such as the Society of Environmental Toxicology and Chemistry (SETAC) and the International Association for Great Lakes Research (IAGLR).

The original project timetable is provided in the project workplan (USEPA, 1997a). At this time (November 26, 1997), project database development has been somewhat slower than anticipated and modelers have only received limited project data. Generally, model results will be ready for review for the first contaminant of interest in about one year after release of project data including submission of atmospheric and tributary loadings. After two years, a draft project report should be ready for review. It is anticipated that the formal modeling aspects of the project will be completed near the end of FY-2000. Journal articles and presentations at scientific meetings will likely occur during and after the project.

Project Personnel

Modeling personnel are located at three primary participating laboratories:

1. The Office of Research and Development, National Health and Environmental Effects Research Laboratory, Mid-Continent Ecology Division-Duluth, Community-Based Science Support Staff, Large Lakes Research Station, Grosse Ile, Michigan.

2. National Oceanic and Atmospheric Administration, Air Resource Laboratory, Atmospheric Sciences Modeling Division, Research Triangle Park, North Carolina (under Interagency Agreement (IAG) with USEPA, National Exposure Research Laboratory).

3. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan (under IAG with CBSSS).

4. U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi.

In addition, the Modeling Workgroup includes personnel from state government agencies, Canadian Global Emissions Interpretation Centre (CGEIC), Mississauga, Ontario, Canada; the consulting firm, Limno-Tech, Inc., Ann Arbor, Michigan; Gerald Keeler, University of Michigan; Keri Hornbuckle and Joseph DePinto, State University of New York (SUNY) at Buffalo; and Steven Eisenreich, Rutgers University. The USEPA-Grosse Ile group includes on-site contractor modelers and programmers from SoBran, Inc., PAI/SAIC and OAO Corporation.

Vitae for all primary modelers and support personnel are included in Appendix B. All primary modelers have considerable training and experience in their areas of expertise. Many are regarded as international experts and have excellent publication records. An important note is that the water modelers have spent most of their careers working on various aspects of the Great Lakes and understanding and modeling Great Lakes phenomena.

Key Support Facilities and Services

Community-Based Science Support Staff, Large Lakes Research Station, Grosse Ile, Michigan

This research facility located on Grosse Ile, Michigan houses state-of-the-art computer and laboratory equipment. Modelers use PCs (with Pentium processors) and Macintoshes (power PC processors). They access several on-site UNIX-based workstations via Ethernet. These include two DECAlpha servers, two DECAlpha workstations, a Sun Sparc10 workstation, two Sun Sparc2 workstations, and a Silicon Graphics workstation. In addition, they are linked via T1 connection to the Internet to other agency computers including the Cray supercomputer in Bay City, Michigan. Two RAID disk arrays provide 50 GB of local data storage. Model code development is supported by an on-site contractor programming staff from OAO Corporation.

Grosse Ile computer software resources include FORTRAN compilers and debugging tools. Other software includes: Oracle database, ArcInfo/ArcView GIS, AVS 2- and 3-b visualization, Excel/QuattroPro spreadsheets, WordPerfect wordprocessing, and IDL. A "modeling support" system is being developed which will expedite development of models and analysis and visualization results. Model code is managed using the Revision Control System (RCS) (Appendix C).

National Exposure Research Laboratory, Atmospheric Modeling Division (AMD), Research Triangle Park, North Carolina

The computer/networking infrastructure available to AMD modelers provides interoperability and connectivity to allow transparent access to distributed high-performance computational resources from the user's desktop. The distributed resources appear to the user to be a single computing environment with data accessible via the facilities of Network Information Service (NIS), Network File System (NFS), and Automount. The user desktop hardware is typically composed of Sun workstations, Sun Sparc 10/40, Sun Sparc 20/50, and Sun UltraSparc II's. -- although a few users have chosen Macintoshes (Power PC processors) or PCs (with Pentium Processors). In addition to the desktop computing capabilities, more powerful servers are also transparently available to all modelers: a general interactive server (Sun UltraSparc II with creator 3D graphics), a model execution server (DEC AlphaServer 2100 with 4-21064 CPUs (190 Mhz)), 512 Mbytes memory, 50 GB disk, anonymous FTP server, primary and backup Network Information Servers, file and e-mail server -- (Sun Sparc 10/40), application server (Sun UltraSparc II), OSF application server (DEC AlphaServer 2100 with 2-21064 CPUs (275 Mhz)), archive server (200+ GB disk and 300 GB near-line tape storage), Single Instruction Multiple Data array computer (4096 processor MasPar with DEC-station front-end), visualization server (SGI Indigo-2 with Extreme graphics subsystem), a public access server (Sun Sparc 10/40). In addition to the local computing infrastructure, the modelers have access to USEPA's National Environmental Supercomputing Center (NESC) in Bay City, Michigan via T3 connection. Model code development is done in-house with some contract programming support from OAO Corporation. A modeling framework development, Models-3, is done by contract systems development system from Science Applications International Corporation (SAIC).

AMD computer software resources include D, C++, JAVA, FORTRAN 77 & 90, Basic, and Perl compilers; SAS and National Center for Atmospheric Research (NCAR) graphics libraries, Digital Extended Math Library, and NetCDF libraries, Parallel Virtual Machine (PVM), KAP optimizer parallel computing tools; Oracle and ObjectStore data management systems; AVS, NCSA Collage, Fis5D, Package for Analysis and Visualization of Environmental Data (PAVE) visualization packages; SAS, Arc/Info, and Mathematics; Lotus 123, WordPerfect, LaTEX; WABI and SoftWindows emulation environment for Microsoft Windows; HTML publishing and Internet access tools; Kermit, FTP, TN3270, x3270 communication tools. Model code is currently managed using SCCS, but a transition is underway to CVS for code management.

NOAA, Great Lakes Environmental Research Laboratory (GLERL), Ann Arbor, Michigan

The computer facilities at GLERL are being used for the hydrodynamic and wind wave modeling components of the Lake Michigan Mass Balance Modeling Program. Modelers at GLERL have access to UNIX workstations (HP C160, HP 715/100) and an HP K200 SMP computer with 4 PA-RISC 7200 100 Mhz processors and 256 Mb of shared memory. Over 50 GB of disk space is available for intermediate storage of model results. A DAT/DDS-2 tape backup system allows for long-term storage of large data sets and CDR equipment is available for permanent storage of intermediate size data sets on CDROM. All machines are connected to the Internet via GLERL's T1 connection through the Merit Network.

Software in use for the LMMBP program at GLERL, includes HP's FORTRAN compiler with support for parallel processing on SMP machines, IDL for data analysis and visualization, CorelDraw for presentation graphics, and various wordprocessing and spreadsheet programs. Computer animations of model output in the FLC animation file format can be created and displayed on workstations and PCs using public domain software. GLERL programs for wind interpolation, wind wave calculations, and three-dimensional circulation modeling use a common programming framework developed at GLERL and use a machine-independent industry standard for compact storage of numerical output (XDR format).

Wisconsin Department of Natural Resources, Madison, Wisconsin

The computing facilities located at the Wisconsin Department of Natural Resources (WDNR) headquarters office in Madison, Wisconsin are being used for tributary model development. Modelers at WDNR have access to a DECAlpha Station 500 UNIX workstation running a 500 Mhz, EV4 Alpha processor with 256 Mb of RAM and 10 GB of disk storage. A 4 mm DAT tape system allows for file backup and long-term storage. This platform is connected to the internet through WDNR's T1 connection. Additional in-house computing facilities include Windows-based Intel platforms (80486 and Pentium II processors) and Apple Macintosh personal computers.

WDNR computer software resources include FORTRAN compilers and debugging tools. Other software includes: ArcInfo/ArcView GIS, Excel, and Quattro spreadsheets, and Word and WordPerfect wordprocessing. Model code will be managed using the RCS.

U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi

Modelers at Waterway Experiment Station (WES) use PCs, a DECAlpha workstation, and a Silicon Graphics INDY workstation.

The modeling team communicates via the Internet for e-mail and for transferring data sets and code. Monthly teleconferences are held to review project status and discuss important issues.

The University of Michigan, Air Quality Laboratory, Ann Arbor, Michigan

The University of Michigan, Air Quality Laboratory (UMAQL) is serviced by two major computing resources centers on the campus of the University of Michigan: the Computer Aided Engineering Network (CAEN) and the Information Technology Division (ITD). CAEN supports more than three thousand workstations, personal computers, and specialized research computers. Among these computers are those that may be found in CAEN's engineering labs, including SUN and Hewlett-Packard workstations and Apple Macintosh and IBM-compatible personal computers. The CAEN also houses the Center for Parallel Computing which contains IBM, Convex and Kendall Square Research parallel supercomputers. The ITD provides computing services to the remainder of the University of Michigan campus.

The University of Michigan is directly connected to two regional Internet providers, MichNet and CICNet. MichNet is a network administered by Merit Network, Inc., which connects Michigan educational institutions to a backbone network service provided by MCI. CICNet is a network that connects several Midwest educational institutions together. Together, these networks provide the University of Michigan's connectivity to the outside world.

The University of Michigan's computing facilities provide state-of-the-art support for the UMAQL and other research interests on campus. Among the services available for this project are the Advanced Visualization Laboratory and the ITD Videoconferencing Service. The Advanced Visualization Laboratory (AVL) at the University of Michigan is designed to facilitate the analysis and display of scientific data and imagery. The AVL provides resources that allow users to easily work with both video and computer based images and to be able to save and display those images in a variety of formats (video, computer, color prints, and color slides).

Computer resources within the UMAQL include a SUN SparcStation/10 for ingestion, display, analysis, and archive of real-time meteorological data from the National Weather Service (NWS) and NOAA. The UMAQL houses one SUN SparcStation IPC (with one gigabyte local storage capacity, plus a 750 megabyte external storage device), one SUN SparcStation/20 (with a 4.2 gigabyte external storage device), and one SUN UltraSparc 167MHz workstation. Finally, the UMAQL owns an Exabyte 8505 high density tape drive, which is needed to read the WSR-88D radar data which will be used to compute wet-deposition estimates for the project.

The UMAQL software library contains all of the necessary tools to carry out the tasks as described above. Basic statistical analyses will be carried out using the SAS 6.12 Statistical Software Package. This package will allow for sophisticated multivariate correlation analyses, as well as the use of various hypothesis testing approaches. The UMAQL software library also contains the most recent version of the Regional Atmospheric Modeling Systems

(RAMS), Version 3B. Further, a Lagrangian particle dispersion model and airmass trajectory model (HY-SPLIT) has been recently updated and will be available for this project.

In addition, the University of Michigan has a site license for the NCAR Graphic software package, which will allow for the detailed graphical presentation of the deposition model output. Also, advanced data display software available at the University of Michigan will allow for the presentation of transport simulations in an animated, three-dimensional format.

Modeling Approach

The general approach for developing models for large aquatic systems is described in the Green Bay Final Report (Richardson *et al*., 1997). This approach has been followed during the initial phases of the Lake Michigan project:

1. Determine specific management questions.

2. Define the appropriate modeling framework needed to address these questions.

3. Propose alternative modeling/project designs for management review for narrow range of expectations and costs.

4. Using historical data and current modeling theory, construct a preliminary screening model to test the sensitivity of various model components.

5. Perform statistical analyses of historical data to determine optimal sampling designs.

6. Make specific sampling design recommendations.

7. Maintain a continuing dialog with other committees on technical issues.

8. Work with investigators who collect and analyzed samples to conduct a "data quality assessment" to evaluate project data. Evaluate data replicates and other QA notations to determine appropriate interpretation of data.

9. Develop and test the final models. Testing includes comparison of calculated concentrations to field data and adjusting model parameters within appropriate and justifiable ranges to obtain a fit within plus/minus one standard error of data mean.

10. Provide answers to specific management questions.

11. Document models and results.

Steps 1 through 6 have been completed and step 8 continues. Step 9, develop and test final models, is presented in detail in the Modeling Workplan (Appendix A). The Lake Michigan "Model" will embody a set of linked submodels. The submodels are depicted in Figure 2 and include:

Water Models

1. Computational Transport Models. These models, which predict physical motion and transport in the lake in response to gravitational and frictional forces (primarily wind), are applied on a common 5 km square horizontal grid for Lake Michigan. They include:

   A. The hydrodynamic model (Princeton Ocean Model (POM)) solves the equations of continuity, momentum, and energy balance to predict three-dimensional velocity, dispersivity, and temperature distributions in the lake. The prediction of water motion by the hydrodynamic model serves as the transport foundation for all mass balance simulations.

   B. The surface wave model (GLERL/Donelan Wave Model) predicts the height, period, and direction of surface waves based upon momentum balance. Surface waves are important forcing functions for sediment resuspension, and also influence the rate of chemical exchange between water and air.

   C. The sediment transport model (SEDZL) predicts the settling, resuspension, and deposition of coarse, medium, and fine-grained sediments based upon the coupling of hydrodynamic and mass balance computations.

Vertical particle transport fluxes predicted by SEDZL will be used as input to the contaminant transport and fate model, specifically, as sediment resuspension fluxes and settling velocities.

2. Mass Balance Models. These models predict the concentrations of chemical constituents in water column and sediment, based upon mass balance equations using a common three-dimensional segmentation and computational framework. They integrate loading estimates for the atmosphere and tributaries, initial conditions in sediment and water column, physical transport, and chemical-specific kinetic processes. They include:

   A. The eutrophication/sorbent dynamics model integrates organic carbon primary productivity and transformation processes, based upon a eutrophication modeling framework, with sediment transport fluxes, to predict the transport and transformation of particulate organic carbon (POC). POC is the primary sorbent phase for hydrophobic organic chemicals in aquatic ecosystems, therefore, its simulation in the mass balance framework for Lake Michigan has been enhanced.

   B. The contaminant transport and fate model predicts toxic chemical concentrations in the water column and sediment. This model shares the computational and many conceptual features with the eutrophication/sorbent dynamics model. The toxic chemicals are added as state variables, which partition between aqueous and several operational sorbent phases in each spatial compartment. Also added are volatile exchange between water and air, and chemical-specific transformation processes. The contaminant transport and fate model will also be used to predict bioavailable chemical concentrations to be used as exposure input to the food web bioaccumulation model.

3. Bioaccumulation and Ecosystem Models

   A. Food Web Bioaccumulation Model: The food web model simulates the bioaccumulation of toxic chemicals leading to the prediction of chemical concentrations in lake trout and coho salmon. The model is based upon a single-component chemical mass balance for a fish.

   B. The Ecosystem Model will build on the existing Great Lakes eutrophication models and incorporate more biological detail. This will be done to reinforce the understanding of ecosystem modification impacts on energy and chemical cycling. Because this is a recent addition to the project, details for this work will be incorporated as they become more clear.

Air Models

Atmospheric fluxes of toxic chemicals over the large surface areas of the Great Lakes and Lake Michigan, in particular, are major contributors to the mass balance. The screening model calculations done using the MICHTOX model (Endicott *et al*., 1992) indicate that over the long-term atmospheric fluxes to Lake Michigan will eventually control PCB concentrations in lake trout. Although the original intent of the project was to develop source-receptor models for each contaminant, it was determined that insufficient information exists for the sources of PCBs and TNC. Therefore, the atmospheric modeling efforts will focus on atrazine as the sources are known and data and models for source estimation exist. Also, there will be sufficient data for mercury to at least make an attempt to model this chemical. Loadings for PCBs and TNC will be estimates from interpolation of field measurements. In the long-term, it should be understood that atmospheric vapor phase PCB concentration over the lake may determine the eventual concentration in lake trout. MICHTOX screening results indicate that if the vapor phase concentration remain at the present estimated levels of 0.24 ng/m^3, the lake trout concentration will reach a steady-state concentration of 1 mg/kg. So in the long run it will be important to determine the sources (global, regional, and local) of PCBs if a rational control program is to be determined and instituted. If sufficient source information becomes available in the future, then coupling PCB air-water models might be attempted to simulate the bi-directional transfer and feedback of contaminant mass balances for air and water. Again, for this project the

focus of the air modeling will be atrazine and mercury.

The original intent for the project was to develop a coupled air-water model. However, it was determined at the Detroit, Michigan, Air/Water Workshop in June 1995, that because of the time scale differences between air and water processes, this was not necessary. Rather the air models will be run independently and the output will be input to the water models. Because water quality models usually span time frames of seasons to years and air models simulate periods of days or weeks, the air models will be used to simulate important depositional periods. The climatology and statistical methods will then be used to estimate atmospheric inputs on the scale of seasons to years. The model outputs include wet and dry deposition contaminant fluxes and near surface atmospheric concentration. These will be used to define input atmospheric loads and gradient for gas exchange for the water quality models. The specific air models include:

1. Regional Particulate Model (RPM): An engineering version of the RPM model adapted for atrazine will simulate transport above the watershed and lake, the gas/particle partitioning and transformation of atrazine in the atmosphere, and the significant deposition and exchange processes with the watershed and lake.

2. Regional Acid Deposition Model (RADM): Simulations will be used to determine the total particulate mass loadings and particle size distribution which affect the behavior of particulate atrazine.

3. Penn State University (PSU)/NCAR Mesoscale Model-Generation 5 (MM5): Generates diagnostic simulations of wind temperature, humidity, cloud cover, and other meteorological variables. This technique continually corrects certain model variables toward observed values during the simulation to control errors. MM5 results are used in the RADM and RPM models.

Mercury Emissions Inventory

An inventory of anthropogenic sources of atmospheric mercury has been developed and described in USEPA's Mercury Study Report to Congress as mandated in Section 112(n)(1)(B) of the Clean Air Act, as amended in 1990. This inventory accounts for a variety of industrial, commercial, and residential source types within all 50 states of the United States. It has been subjected to rigorous peer review both inside and outside USEPA and has been judged to accurately describe the total mass and spatial distribution of mercury emitted to the atmosphere from anthropogenic sources in the U.S. This emission inventory has been used to support regional-scale atmospheric mercury deposition modeling, the results of which are also described in USEPA's Mercury Study Report to Congress. This regional-scale modeling showed that, in addition to total mass, the chemical and physical forms of mercury emissions are important in determining the patterns and intensity of mercury deposition to the surface. Studies of the chemical and physical forms of mercury emissions from various source types are currently ongoing.

Atmospheric mercury emissions from natural sources and from anthropogenically contaminated soils and water bodies are not as well understood as are the current direct anthropogenic emissions to air. It can be reasonably assumed that these natural and recycled emissions are mostly in the form of elemental mercury gas due to the relatively high vapor pressure of elemental mercury versus its oxidized compounds. However, the total mass of natural and recycled mercury emissions and the spatial distribution of those emissions are not confidently known at this time. It may be possible to model natural and recycled mercury in the form of a global-scale background concentration if it can be determined that no such emissions are significantly concentrated near Lake Michigan.

Anthropogenic emissions of mercury from sources in Canada are currently being surveyed by Canadian federal and provincial governments and preliminary inventories from this effort are now available. An accurate emission inventory for Canada including chemical and physical form definitions will be required for an accurate modeling assessment of total mercury deposition to Lake Michigan.

Emissions of mercury from anthropogenic sources in Mexico and more distant countries might be adequately accounted for by the global-scale background concentration also used to account for natural and recycled emissions. It is generally thought that oxidized mercury emissions will mostly deposit to the surface or convert to the elemental form within the transport distance from

Mexico to Lake Michigan. Atmospheric mixing of the remaining mercury from these distant anthropogenic sources could make their mercury plumes indistinguishable from global-scale emissions. We currently do not have a complete understanding of the global-scale transport of atmospheric mercury. Thus, the concept of a nearly constant global background concentration of elemental mercury gas may be invalid.

However, in the absence of comprehensive emission inventories for all industrial nations and global-scale atmospheric models to use them, we are forced to employ some form of background concentration or constant boundary influx concentration in our modeling of atmospheric mercury deposition to Lake Michigan.

Quality Control

Quality control is defined as the process by which QA is implemented. All project modelers will conform to the following guidelines:

1. All modeling activities including data interpretation, load calculations or other related computational activities are subject to audit and/or peer review so careful written and electronic records should be kept for all aspects of model development and application.

2. Written rationale will be provided for selection of models or versions of models like WASP4 or WASP-IPX, SEDZL, etc.

3. As modeling computer programs are modified, the code will be checked and a written record made as to how the code is known to work (i.e., hand calculation checks, checks against other models, etc.). This should include input and output, if appropriate or results of external calculations used to confirm code.

4. If historical data are used, a written record on where this was obtained and any information on its quality will be maintained. A written record on where this information is located on a computer or server will be maintained.

5. If new theory is incorporated into the model framework, references for the theory and how it is implemented in any computer code will be documented.

6. All new and modified computer codes will be documented. This should include internal documentation, as revision notes in program headers, and external documentation, in user's guides and supplements.

Audits of each modelers work will be conducted periodically by the Agency QA auditing team, the project QA officer, MED-Duluth QA officer or one or more of their designees.

Modelers will be asked to provide verbal status reports of their work at the monthly modeling workgroup teleconferences. Finally, detailed modeling documentation will be made available to members of the Science Review Panel (see peer review section below) as necessary.

The ability of computer code to represent model theory accurately will be assured by following rigorous programming protocols including documentation within code. Specific tests will be required of all models and revisions to ensure that fundamental operations are verified. These include continuity and mass conservation checks. These also include testing of numerical stability and convergence properties of model code algorithms, if appropriate. Model results will be generally checked by comparing results to those obtained by other models and by comparison to manual calculations. Visualization of model results will assist in determining whether model simulations are realistic. Model calculations will be compared to actual field data. If adjustments to model parameters have to be made to obtain a "fit" to the data, modelers will provide a rigorous explanation and justification that must agree with scientific knowledge and with process rates within reasonable ranges as found in the literature.

Models will be deemed acceptable when they are able to simulate field data within plus/minus one standard error. The standard error will be determined by accepted statistical methods by stratifying data appropriately in time and space. For cases in which model predictions do not match the spatial/temporal resolution of data, the appropriate averaging of either data or predictions will be determined and justified. The appropriate scales will be

determined by the modeling team in consultation with the Science Review Panel.

Data Quality

Data Quality Assessment

Both project-generated and non-project-generated data will be used for model development and calibration. The QA procedures for project-generated data and database development have been discussed in this document and elsewhere. All analytical data for the model's target analytes and most supporting data will have been verified through the RDMQ process before release to the modelers.

The Project QA Plan (USEPA, 1997b) provides the QA program and process, organizational structure, data quality objectives, implementation of the QA Program and information management guidelines for the LMMBP. The process calls for approved workplans, SOPs, and QA plans for each aspect of field collections and laboratory procedures. Rigorous examination of precision, accuracy, completeness, representativeness, detectability, and comparability is and will be conducted on project-generated data by QA managers. These will not only include examination of the data itself but also technical systems audits, data quality audits, management systems reviews, and performance evaluations. Project-generated data will be verified and validated using the RDMQ process which controls measurement uncertainty, evaluates data, and flags or codes data against various criteria. This portion of the QA process is also associated with final database construction. The final database repository for the LMMBP will be Oracle and will contain all formatted, verified, and validated project-generated data with associated information (USEPA, 1995b, 1997f). Modelers will cross-check the data for bias, outliers, normality, completeness, precision, accuracy, and any other potential problems. Determinations will also be made using best professional judgement as to selecting field replicates in different situations.

Non-project-generated data may be obtained from either published or unpublished sources. The published data (including those from gray literature) will have had some degree or form of peer review. Certainly there is a wide range of review quality from journal to journal. However, given that some degree of review has been performed, databases are often obtained directly from authors or from on-line databases. These are generally examined by modelers as part of a data quality assessment. In the case of databases that have not been published, these databases are also examined in light of a data quality assessment.

Database Tracking

A database tracking system has been instituted by the CBSSS, Grosse Ile, for modeling systems. This system employs a single contract person for data being received. One contact person logs in routine information about the data and coordinates its use. The process provides updated versions if changes occur from the GLNPO database. The second component of tracking involves versions which have been assessed and completed for modeling purposes. The datasets are X-Y-Z set for model input (see below).

Model and Input/Output File Tracking

A system for tracking models, input files, and output files has been developed by CBSSS, Grosse Ile. This system is referred to as "RCS". During model calibration and testing, various versions of each were used to examine model performance. This system coordinates the version of each model, input, and output files so that any can be recalled, run, or examined. Associated documentation of these aspects are also developed as part of the tracking and modeling system.

Record Keeping

All records including modelers notebooks and electronic files will be maintained according to Agency standards as defined by the USEPA Office of Information Resources Management (http://www.USEPA.gov/irmoli) Federal Information Processing Standards (FIPS), http://www.nist.gov/itl/div879/pubs and professional standards like ANSI/IEEE Standard 730-1989 for Software Quality Assurance Plans.

These laboratory notebooks and electronic files will be maintained by each modeler and turned over to the laboratory QA officer upon completion of the project. Electronic files containing documentation of model testing, calibration, and validation will be maintained by each modeler and transferred to a central project archive

as designated by the QA official.

Data Usage

When a great amount of data are collected for various media such as in this study, a considerable number of autonomous results will be reported and/or published. However, this data have been specifically collected and analyzed for the purposes of the LMMBP, and mathematical modeling. Undoubtedly other uses will be attempted but data have not been specifically obtained for these purposes. Modelers will use the data for establishing relationships and associations, defining processes and quantifying process rates, and checking existing model input files, relationships, and rates.

The above aspects pertain to model calibration and testing. This is an interactive process and requires considerable data. A final step in the calibration process is to determine the agreement between the observed and computed conditions.

Peer Review

Peer review is an essential component to any successful and credible scientific/modeling endeavor. Model development and application is a very complex process and there are many debatable issues and many approaches that could be taken. Peer reviews provide an objective means to arrive at scientific consensus on a number of these issues as well as providing judgements on scientific credibility.

USEPA has provided guidance for conducting peer review of environmental regulatory modeling projects (USEPA, 1994). This guidance acknowledges the utility of peer reviews for all phases of the modeling work from planning through application. The Agency policy also points out that the guidance does not directly address models developed for reasons other than to support regulatory decision-making. Therefore, research models developed for and used exclusively within a research program should receive peer review by scientific colleagues, senior scientists, managers, and by reviewers for refereed journals. If the research model evolves to a point that decisions may be made as a result of its use, then a formal Agency peer review would be appropriate, if not mandatory. Because the LMMBP is being conducted in support of the Lake Michigan Lake-wide Management Plan, all aspects of the modeling are deemed to require peer review.

Agency guidance offers three mechanisms for accomplishing external peer review:

1. Using an *ad hoc* technical panel of at least three scientists;

2. Using an established external peer review mechanism such as the Science Advisory Board or Science Advisory Panel; or

3. Holding a technical workshop.

Further guidance is provided for determining when and by what mechanisms to initiate an external peer reviews and how to document them. The guidance does not appear to take into consideration the use of multiple models, as being done for Lake Michigan. So when referring to “the model” it is assumed that it applies to the entire modeling framework provided in the LMMBP Modeling Workplan.

The LMMBP Modeling Workplan was reviewed externally, but not by a formal peer review panel. It was incorporated into the project workplan which was distributed to a large number of experts and to the public. Comments were received and adjustments were made accordingly. Before any substantial modeling efforts begin, a peer review panel should be selected and a review convened.

All aspects of Lake Michigan model development and application will be reviewed by a “Science Review Panel”. The panel will consist of well-known scientists and engineers who have experience in developing and applying models but who have no direct contact with the project. This will ensure objectivity and avoid any conflict of interest. The panel will meet at least semi-annually and more frequently if needed. The initial review should be scheduled for February 1998.

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Chapter 3
Individual Model Quality Assurance Plans

Computational Transport

Hydrodynamic Model of Lake Michigan

Project Officer: Ronald Rossmann and Douglas Endicott, USEPA, LLRS
Principal Modeler: David J. Scwab, NOAA
Support Modeler: Dmitry Beletsky, Cooperative Institute for Limnology and Ecosystems Research (CILER)

A. Model Description

1. Background Information - The numerical circulation model used in this task is a three-dimensional ocean circulation model developed at NOAA's Geophysical Fluid Dynamics Laboratory at Princeton University for coastal ocean applications by Blumberg and Mellor (1987) and subsequently adapted for Great Lakes use at GLERL (Schwab and Bedford, 1994; O'Connor and Schwab, 1994). The model is driven by time-dependent surface boundary conditions for wind stress and heat flux. The physical parameters predicted by the model are the three-dimensional velocity distributions, the temperature field, and the free surface water level. The main features of the model are:

   - Fully three-dimensional nonlinear Navier-Stokes equations
   - Flux form of equations
   - Boussinesq and hydrostatic approximations
   - Free upper surface with barotropic (external) mode
   - Baroclinic (internal) mode
   - Turbulence model for vertical mixing
   - Terrian following vertical coordinates (<sigma>-coordinate)
   - Generalized orthogonal horizontal coordinates
   - Smagorinsky horizontal diffusion
   - Leapfrog (centered in space and time)
   - Implicit scheme for vertical mixing
   - Arakawa-C staggered grid
   - FORTRAN code optimized for vectorization.

   The terrain following vertical coordinate system (sigma-coordinate) replaces the vertical coordinate, z, with a normalized vertical coordinate, sigma = z/d, where d is the local depth. The advantage of this system is that in the transformed coordinate system, the bottom corresponds to a uniform value of the vertical coordinate (sigma = -1), thus simplifying the governing transport and continuity equations. The disadvantage is that an extra term is introduced in the pressure gradient involving the gradient of bottom topography. As Haney (1991) has shown, the truncation error in the finite difference representation of this term can be considerable near steep topography. We have been careful in the design of numerical grids for the Great Lakes to minimize these problems. Although the current version of the model can incorporate a curvilinear, coastline-following coordinate system, this feature is not used in the Great Lakes version. We felt that the additional complication of a curvilinear coordinate system in the interpolation and analysis of model results were not justified by the potential for increased accuracy in the hydrodynamic model.

2. Data Quality - Two data sources will be used to calibrate the Lake Michigan model. Heat flux and momentum flux forcing functions will be

estimated from the NWS observations and buoy data from 1982-83. This data has been used successfully in the USACOE Wave Information Study for the Great Lakes (Hubertz *et al*., 1991). Model results for the 1982-83 simulation will be calibrated against currents and temperatures measured by GLERL during the 1982-83 field program. These data were collected with state-of-the-art oceanographic instrumentation from an extensive deployment array and then edited and analyzed at GLERL (Gottlieb *et al*., 1989).

Meteorological data for the 1994 simulation will be obtained from the NWS stations described above as well as additional marine observations from U.S. Coast Guard (USCG) stations and ships of opportunity in Lake Michigan. These data are routinely collected and quality-controlled at the Cleveland Weather Service Forecast Office. In addition, data from several meteorological stations in the LMMBP air sampling network around Lake Michigan will be used. The QA/QC procedures for these data are described in the air sampling network plan.

B. Model Development

1. Code Development and Maintenance - The code used in the hydrodynamic circulation model is based on the FORTRAN code of the POM as described in Mellor (1996). The adaptations made for application to the Great Lakes are described in Schwab and Bedford (1994) and within the code itself.

2. Model Documentation - A complete description of the model equations, underlying assumptions, boundary conditions, and numerical methods is contained in Mellor (1996). A practical operator's guide for the Princeton model was compiled by O'Connor (1991) and was used extensively in the development of the Great Lakes version of the model. The scientific basis for adaptations of the model to the Great Lakes is described in Schwab and Bedford (1994) and O'Connor and Schwab (1994).

3. Code Verification - Hydrodynamic modeling codes are typically verified with tests against analytic solutions and by sensitivity analysis. The code used in this task has been tested for several analytical cases including external and internal seiches, logarithmic boundary layer, horizontal and vertical diffusion, thermal structure development, and barotropic wind-driven circulation (O'Connor and Schwab, 1994; Schwab *et al*., 1994). All tests indicate the model is coded correctly.

4. Code Documentation - The FORTRAN code for the model comprises approximately 4000 lines of code and comments. The code has been developed over a period of 10 years at Princeton and adheres to modern programming techniques and standards. In addition to extensive internal documentation, a comprehensive user's guide is available (Mellor, 1996) as well as an operator's manual (O'Connor, 1991). Documentation of specific adaptations made for the Great Lakes version are described by Schwab and Bedford (1994).

5. Model Calibration/Validation and Uncertainty - The POM has been used extensively for coastal and estuarine applications, including the Middle Atlantic Bight, the South Atlantic Bight, the California Shelf, the Santa Barbara Channel, and New York Harbor. The Great Lakes version is used operationally in the Great Lakes Forecasting System (Bedford and Schwab, 1990; Schwab and Bedford, 1994) for Lake Erie. Extensive validation tests with observed currents, water level fluctuations, and surface temperature distributions have been carried out in the development of the Great Lakes Forecasting System Model validation against 1982-83 current and water temperature measurements in Lake Michigan is also a part of this task.

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Wind Wave Model for Lake Michigan

Project Officer: Ronald Rossmann and Douglas Endicott, USEPA, LLRS
Principal Modeler: David J. Schwab, NOAA
Support Modeler: Dmitry Beletsky, CILER

A. Model Description

1. Background Information - The wind wave model used in this task is the GLERL/Donelan parametric wind wave model developed by Schwab *et al*. (1984a,b). This is a numerical finite-difference solution to the two-dimensional wave momentum conservation equation. The wave energy spectrum is parameterized at each point on a rectilinear computational grid in terms of total wave energy, peak energy period, and predominant wave direction. Momentum is transferred from the wind to the waves using Donelan's (1979) formulation which depends on the difference between the phase velocity of the waves and the local wind velocity.

   The principal assumptions of the model are:

   - Equipartition of kinetic and potential wave energy
   - Waves propagate according to deep water theory
   - Wave directional spreading follows a cosine squared law
   - The JONSWAP (Hasselman *et al*., 1973) spectral shape is used
   - The wave spectrum equilibrium range parameter follows the JONSWAP empirical dependence on nondimensional fetch
   - Only actively generated waves are considered. The "fossil" wave field discussed in Schwab *et al*. (1994a) is not employed.

   This model has been successfully applied to Lake Erie (Schwab *et al*., 1984a) and Lake Michigan (Liu *et al*., 1984), as well as the Baltic Sea and several other lakes and embayments around the

world. The NWS has used this model for routine lake wave forecasting on all five Great Lakes since 1992 (Johnson *et al*., 1992).

2. Model Parameters and How They Will Be Specified - The empirical relations between wave energy, wave period, and nondimensional fetch resulting from the JONSWAP experiment (Hasselmann *et al*., 1973) were developed independently of the model and will not be adjusted for calibration. The parameterization of the momentum transfer from the wind to the waves (Donelan, 1979) includes an empirical constant specifying the percentage of wind stress retained by the waves which can be adjusted for different types of wind input (i.e., ship reports, shore stations, buoys, etc.). This parameter can vary slightly depending on the particular combination of types of wind reports and lake geometry for a particular application. We have adjusted this parameter to optimize the comparison between wave model predictions and wave observations from NDBC buoys in Lake Michigan during the study years (1982-83 and 1994-95).

   Meteorological data to supply wind forcing for the 1982-83 and 1994-95 simulations were obtained from the NWS weather stations and buoys as well as additional marine observations from the USCG stations and ships of opportunity in Lake Michigan. These data are routinely collected and quality-controlled at the Cleveland Weather Service Forecast Office. In addition, data from several meteorological stations in the LMMBP air sampling network around Lake Michigan were used. The QA/QC procedures for these data are described in the air sampling network plan.

B. Model Development

1. Code Development and Maintenance - The code used in the wind wave model is based on the FORTRAN code of Schwab *et al*. (1984b). The adaptations made for applications to the LMMBP are described above and within the code itself.

2. Model Documentation - A complete description of the model equations, underlying assumptions, boundary conditions, and numerical methods is contained in Schwab *et al*. (1984a, 1986). The original source code for the model is presented in Schwab *et al*. (1984b). Additional documentation of adaptations particular to the LMMBP will be described in the final project report and in the source code itself.

3. Code Verification - Hydrodynamic modeling codes are typically verified with tests against analytic solutions and by sensitivity analyses. The code used in this task has been tested for several idealized cases including purely fetch-limited conditions, duration-limited conditions, and several tests of directional divergence, in various geometries (Schwab *et al*., 1984a). All tests indicate the model is coded correctly.

4. Code Documentation - The FORTRAN code for the model comprises approximately 1200 lines of code and comments. The code has been developed over a period of 10 years at GLERL and adheres to modern programming techniques and standards. In addition to extensive internal documentation, a user's guide is available (Schwab *et al*., 1984b). Documentation of specific adaptations made for the LMMBP are described in the code itself and in the final project report.

5. Model Calibration/Validation and Uncertainty - The GLERL/Donelan Wave Model has been used extensively for Great Lakes applications. Schwab *et al*. (1984a) compared wave model results to wave measurements from an instrumented tower in Lake Erie and found root mean square differences on the order of 0.2 m for wave height and 1 sec for wave period. Liu *et al*. (1984) showed a high correlation between model results and lake-wide synoptic wave height measurements from an airborne laser altimeter in Lake Michigan. The GLERL/Donelan model is also used operationally by the NWS (Johnson *et al*., 1992) and has proven to be highly accurate when wind forecasts are accurate.

   Model calibration against wave buoy measurements in 1982-83 (NDBC 45002 and 45007) and model validation against wave buoy

measurements in 1994-95 (NDBC 45002, 45007, and 45010) in Lake Michigan will also be carried out as part of this task.

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Sediment and Contaminant Transport/SEDZL

Principal Investigator: Douglas Endicott, USEPA, LLRS
Contract Support Programmer: Michael Settles, OAO Corporation
Project Advisor: Joseph Gailani, USACOE

A. Model Description

1. Background Information - The numerical sediment transport model developed at the University of California at Santa Barbara (UCSB), Department of Mechanical and Environmental Engineering by Ziegler and Lick (1986) and subsequently refined for use on the Great Lakes at UCSB and LLRS (USEPA, 1997). SEDZL couples vertically-integrated hydrodynamic and sediment transport equations in the water column to a three-dimensional, time-dependent model of the sediment bed. Transport of three different sediment size-classes can be modeled including fine-grained, cohesive sediments which flocculate during settling. These particles are modeled as the medium size-class. All size-classes can be deposited to and eroded from the sediment bed. The sediment dynamics incorporated into SEDZL are based on valid laboratory and field studies concerning the deposition and resuspension of fine-grained, cohesive sediments (Fukuda and Lick, 1980; Lee *et al*., 1981; Lick, 1992; Tsai and Lick, 1987; Burban *et al*., 1990; Xu, 1991). A brief review of the sediment dynamics used in the model will now be presented; a more detailed discussion can be found in Gailani *et al*., 1993, 1994.

   The medium size-class flocculation and laboratory results have been used to construct an approximate flocculation model (Burban *et al*., 1990). The flocculation model estimates the floc size as a nonlinear function of particle concentration and shear stress. Once floc size has been predicted, then the settling rate of medium size-class sediments is calculated.

   The resuspension properties of fine-grained cohesive sediments differ significantly from noncohesive sediments, i.e., sand. Both size-classes are important for sediment transport in

Lake Michigan. Noncohesive sediment will be resuspended at a constant rate if the sediment bed is subjected to a uniform shear stress greater than a critical value. As long as there is a supply of noncohesive sediment, resuspension will occur. However, laboratory and field experiments clearly indicate that only a finite amount of fine-grained, cohesive sediment can be resuspended under the same conditions (Tsai and Lick, 1987). Based upon these experimental results, the total amount of sediment which can be resuspended at a particular bottom shear stress can be calculated.

SEDZL incorporates a realistic model of the sediment bed structure, which is necessary if the transport processes are to be modeled properly. The sediment bed is three-dimensional, with vertical layers representing post-deposition age (t_d) and increasing compaction with depth. The effects of compaction on resuspension are accounted for by t_d, which increases with depth in the sediment bed. The critical shear stress also increases with depth until $t_d \geq 1$ day after which time it is assumed to be constant. Experimental results have shown that compaction effects begin to become negligible for $t_d > 6$ to 7 days.

A volume integral method was used to derive finite difference equations which are used to numerically solve the vertically-integrated Navier-Stokes and sediment transport equations (Ziegler and Lick, 1986). The equations are solved explicitly, using two time levels. Interior and boundary point equations are second-order accurate, conservative mass and momentum both globally and locally, and boundary conditions are treated correctly. A unique feature of this model is its successful treatment of open boundary conditions (Lick *et al*., 1987).

Vertically integrated hydrodynamic and sediment transport equations have been used in SEDZL in order to simplify the numerical analysis (Ziegler and Lick, 1986) and complexity of the model. These equations are valid approximations for situations where the water is relatively shallow and where the vertical stratification of the water column is weak. These assumptions limit the application of SEDZL to situations where there are no significant vertical gradients in either the sediment concentration or the horizontal velocity. SEDZL has also been applied to water bodies where these assumptions have not been strictly satisfied, and the limitations of the model have been evaluated under these circumstances (Lick *et al*., 1994; Wang *et al*., 1996). Application of SEDZL in Lake Michigan clearly falls in this latter category; the procedures in place to evaluate and ensure model credibility are discussed below (4. Model Calibration/Confirmation and Uncertainty).

2. Model Parameters and Input Data - To run SEDZL, the following parameters and input data must be provided: system bathymetry and boundary geometry, sediment loading rates, wind and wave boundary conditions, hydrodynamic parameters (eddy viscosity, bottom friction coefficient, Nikuradse number), sediment transport parameters (eddy diffusivity, settling velocities), sediment bed properties (critical shear stresses, resuspension flux parameters, and rates of compaction), and initial size-class distribution.

   SEDZL will use the same bathymetry and boundary geometry data for Lake Michigan as is being used by POM. The boundary geometry must be slightly modified to accommodate differences in the treatment of some shoreline features by the two models. These include small islands, small embayments, and narrow peninsulas. Wind and wave boundary conditions are input as temporally- and spatially-varying data, again based upon the same forcing functions used by POM. Wind fields will be adjusted for the effects of winter ice-cover, using data generated by the National Ice Center, Defense Mapping Agency. Other hydrodynamic and sediment transport parameters are calculated using the methods documented in the SEDZL User's Manual (USEPA, 1997).

   Sediment bed properties will be estimated from resuspension tests conducted on sediment samples collected in Lake Michigan (Taylor, 1996) and other locations in the Great Lakes (McNeil *et al*.,

1996). To estimate the variation in resuspension properties in sediment, both spatially and with depth, these parameters will be correlated to measured properties including bulk density and grain size (Roberts *et al*., 1997). *In situ* testing of resuspension properties using a submersible, bottom-resting flume (Hawley, 1991) will provide additional data for sediment bed parameterization.

Sediment loading rates will be estimated for sources including shoreline and bluff erosion, tributary loads, and atmospheric deposition. Shoreline and bluff erosion rates will be estimated using the data of Monteith and Sonzogni (1976) and Colman and Foster (1994). Tributary and atmospheric loading estimates are being provided by other LMMBP investigators, as discussed elsewhere in this Modeling QA Plan. Significant sediment loadings will be input as temporal forcing functions to SEDZL.

3. Data Quality - All data used by this project were collected and manager under strict QA/QC guidance as documented in several project-related reports and described above. See "General Considerations" above.

B. Model Development and Maintenance

1. Code Development and Maintenance - The computer program used to model sediment transport is based on the SEDZL model developed by Ziegler and Lick (1986). Refinement of SEDZL for use on the Great Lakes and for this Project are documented in the User's Guide (USEPA, 1997). The code is written in FORTRAN and follows modern programming conventions. The 27,000-line SEDZL program is stored in 42 FORTRAN files and 92 common block files. Program compilation and linking are controlled using a Makefile. Development and maintenance of the SEDZL program is managed using the RCS operating on Digital UNIX workstations. RCS forces strict revision control; supports check-out, locking, and check-in of individual program files for development; and maintains history and documentation on all changes made to each program and common (include) file.

2. Model and Code Documentation - A User's Guide for SEDZL (USEPA, 1997) is maintained at LLRS. All functional changes made to the model program are incorporated into periodic revision of the User's Guide. Internal documentation is also maintained in the header comments of each program subroutine.

3. Code Verification - The SEDZL model has been verified using several approaches, including numerical testing and tests against analytic solutions (Ziegler and Lick, 1986). The operation of the SEDZL model has also been verified through application to at least 10 different water bodies, which have collectively tested all aspects of model performance. Input/output data for simulations in several of these systems have been maintained as "benchmark" tests which are rerun to confirm model performance after code modification. In this study, SEDZL will also be tested by comparison of vertically-integrated velocity and sediment bed shear stress predictions, to comparable predictions made by POM. In addition, SEDZL sediment resuspension fluxes will be compared to predictions generated by sediment transport models employed by the USACOE-WES, Coastal Engineering Research Center.

4. Model Calibration/Confirmation and Uncertainty - Specific data-collection efforts were supported by the LMMBP for calibration and confirmation of sediment transport predictions. These included shipboard sampling of suspended solids and vertical temperature and transmissivity profiles, vertical sequencing-collection sediment trap deployments (to measure bi-weekly particle settling fluxes), deployments of instrument arrays to measure vertical water column profiles of velocity, temperature, and transmissivity, sediment coring and radiometric analyses (to measure the particle burial flux in the sediment bed, the rate of vertical mixing, and the local sediment focusing factor), and additional physical (i.e., grain size distribution, water

content) and chemical analyses of surficial (0-1 cm) sediments collected at ~180 locations throughout Lake Michigan. *In situ* and laboratory testing of sediment bed resuspension properties using flume devices have already been mentioned, as have the source of data for forcing functions (including wind stresses, surface waves, and solids loading).

The principal calibration variables in SEDZL are the particle settling velocities and the sediment resuspension parameters (critical shear stress and resuspension parameter) which vary in three-dimensions within the sediment bed. Initial estimates for these parameters will be based upon settling velocities calculated from the sediment traps, and resuspension parameters calculated from the flume experiments. Spatial distribution of resuspension parameters will be estimated using sediment grain size and water content as correlating variables. SEDZL calibration will also be based upon parameterization from previous applications (as described in the User's Manual) as well as parameterization used in other models applied to lakes and coastal oceans.

Model predictions will be confirmed in both water column and sediment bed. In the water column, the spatial and temporal distribution of suspended solids concentrations will be the principal confirmation variable. Predicted and measured settling fluxes will also be compared. In the sediment bed, the predicted rate and distribution of solids accumulation will be compared to the sedimentation rates based upon core analyses.

Uncertainty in SEDZL prediction of resuspension fluxes is an important issue, since we intend to use the resuspension fluxes as forcing functions in the contaminant transport and fate model. The two major components of uncertainty are expected to be errors arising from use of vertically-integrated hydrodynamics to compute bed shear stresses, and uncertainty (due to lack of sufficient measurements) in the parameterization of sediment resuspension properties. The first component of uncertainty will be evaluated by comparing SEDZL shear stress predictions to those based upon POM, which computes the three-dimensional distribution of lake currents. This comparison, in terms of residual shear stress, can then be translated into a resuspension flux error. The second component of uncertainty, the parameterization of sediment bed resuspension properties, will be estimated by treating the parameters as variables in a Monte Carlo analysis..

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Hydrodynamic Model Linkage with WASP-IPX

Personnel and contractors at the USACOE-WES have been assisting USEPA personnel in implementing a higher-order transport algorithm in their water quality model (IPX) and developing linkage software between the POM and IPX.

The model design for the LMMBP is based on a linked submodel approach, which, in part, includes hydrodynamics, sediment transport, eutrophication, and contaminants. It is the desire of the USEPA that the hydrodynamic model POM and water quality model IPX linkage task follows the work performed by WQCMB, EL on the Chesapeake Bay Eutrophication Study. The objectives of this research project are to: (1) develop and implement a processor subroutine in the POM hydrodynamic model to provide input geometry, flow and diffusion data for the IPX water quality model; (2) implement and test an ICM-type transport scheme in IPX; (3) perform linkage testing on simplified and prototype grids; and (4) document the linkage methodology and

develop a user's guide. The objective of Task 3 has been to implement and test ICM transport within IPX. A detailed description of the ICM transport methodology including all input and output operations is presented in Cerco and Cole (1995).

Linkage and Quality Assurance Testing

The testing of the linkage methodology was performed utilizing a 20 x 20 x 10 test grid. The POM grid coordinate and depth file and IPX-MT (IPX-Modified Transport) map file are the same as those used during Task 2. The POM hydrodynamic output file was read by IPX-MT and a volume balance was performed. The comparison of POM and IPX-MT grid cell volumes were identical within machine accuracy. ULTIMATE QUICKEST mass conservation testing was performed within IPX-MT. Specifically, uniform concentration and spot dump mass conservation tests were performed. The first set of mass conservation tests utilized a one hour time step in POM with no time averaging performed. This resulted in a two hour hydrodynamic update interval in IPX-MT. Subsequent mass conservation tests were performed utilizing six hour average POM flow data, which resulted in a twelve hour hydrodynamic data update in IPX-MT. During all tests, mass conservation was maintained within machine accuracy.

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Mass Balance Water Quality Models

General Considerations for All Mass Balance Water Quality Models

Project Officer: Douglas Endicott, Kenneth Rygwelski, and William Richardson, USEPA, LLRS
Principal Modelers: Douglas Endicott, Solids and PCBs; Kenneth Rygwelski, Atrazine and Mercury; William Richardson, TNC, Atrazine and Eutrophication

Support Modelers: Xiaomi Zhang, SoBran, Inc., Transport, Solids and General Water Quality; James Pauer, SoBran, Inc., Eutrophication; Victor Bierman, Limno-Tech, Ecosystem

A. Model Descriptions

A series of mass balance models are being developed and applied at the USEPA CBSSS. These are generally referred to as water quality models and utilize the same basic transport fields based upon hydrodynamic and sediment transport simulations. They are dissimilar as they are used to model different chemicals and, therefore, diverge somewhat in their fate processes. The four toxic chemicals are: atrazine, PCBs, mercury and TNC. PCBs and TNC use the same fate model but use separate fate process rates.

These models build upon a specified transport regime. This is being developed independently (described in Chapter 2, above). A special project with the USACOE-WES was initiated to assist in translating the hydrodynamic model velocity and dispersion field into appropriate input as a forcing function to the water quality models. In a similar fashion, sediment resuspension fluxes predicted by the sediment transport model will be translated into resuspension rates for bed sediments in the mass balance models. This, together with specifications of external loading of solids and settling velocities for biotic and abiotic particle classes, will establish a mass balance for solids.

While the solids mass balance is a requirement, it is not sufficient to fully describe the transport of particulate chemicals. It is also necessary to simulate the dynamics of the sorptive phase, which is generally agreed to be organic carbon. Organic carbon is non-conservative, with primary production, transformation, and loss all occurring in the lake. The dynamics of organic carbon sorbents are modeled within a eutrophication model framework.

After the solids/sorbent mass balance model is constructed and calibrated, work can be done to develop the models for toxic chemicals. The appropriate processes governing the fate of each chemical will be considered.

The sections below cover information that apply to all of mass balance models. Specifics will be noted as necessary for later sections describing the QA plans for individual models.

1. Background Information - The Lake Michigan Water Quality models are based on the approach provided in the general USEPA-supported water quality model, Water Analysis Simulation Program (WASP). WASP has a long history and has been developed, applied, and refined over the past 25 years. It was originally developed by Dominic Di Toro, Manhattan College, who received support from USEPA, ORD (Di Toro *et al*., 1983). Modelers at the USEPA LLRS began using the original version of WASP in the mid-1970s. At that time it only ran via support of Manhattan College staff on the New York University (NYU) computer. HydroScience, Inc., an environmental consulting firm also had a proprietary version of the model and was applying it to water bodies throughout the world. Because WASP was difficult to operate remotely, LLRS contracted with HydroScience to formalize the code, document it, and implement it on the USEPA DEC-PDP-11/45 computer at Grosse Ile, Michigan. The user manual was widely distributed and the source code was transferred to the USEPA, Athens, Georgia laboratory where it became a public domain USEPA-supported model at Center for Exposure and Assessment Modeling (CEAM).

   The original WASP models were developed to simulate water quality state-variables for dissolved oxygen and eutrophication. In the late 1970's, hybrids of WASP were developed by Thomann, Di Toro, and Richardson for simulations of solids and partitioned toxic chemicals including PCBs. The Manhattan College version became known as WASTOX and the USEPA version combining the WASP chassis with EXAMS processes became known as ToxiWASP. In the mid-1980's, a project was funded by ORD to consolidate the best of the these two versions into WASP-4. Since then CEAM has revised the model further into WASP-5. Documentation and user manuals are available for all of these versions and the CEAM- supported versions with documentation can be obtained from the Internet via their homepage, http://www.epa.gov/CEAM/ .

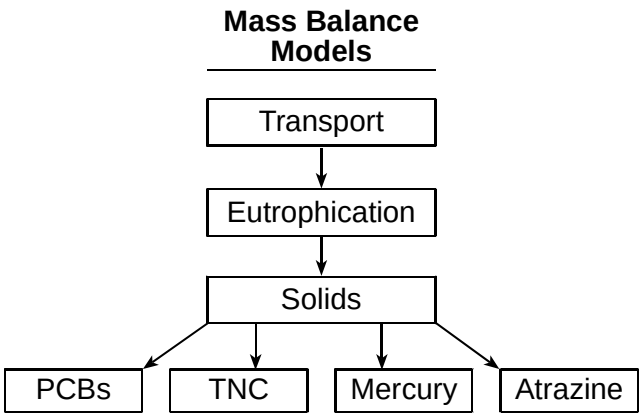

Figure 4. Relationship Between Mass Balance Models.

   While WASP (and its derivatives) has been the primary water quality model employed by USEPA and their cooperators, this framework is being substantially modified to incorporate transport solution algorithms from the USACOE QUAL-ICM model. QUAL-ICM has been applied by the WES as a eutrophication model in numerous studies, most notably Chesapeake Bay and Los Angeles/Long Beach Harbors. QUAL-ICM is being incorporated in the Lake Michigan mass balance models for two reasons. First, the QUICKEST/ULTIMATE (Leonard, 1979, 1991) method for solution of the advective/dispersive transport components of the mass balance equation removes restrictions on segmentation geometry and solution time-step size. These are quite problematic when applying WASP at the high resolution intended for this project. Second, the QUAL-ICM model already incorporates procedures to read hydrodynamic model-generated advective and dispersive transport fields, as well as the necessary mapping

translation between gridded and unstructured segmentation models.

Mass balance models require specification of segment geometry; advective and dispersive transport; boundary concentration for state variables; point and diffuse source loads; kinetic parameters; constants, and time functions; and initial conditions. These input data, together with the general mass balance equations and the specific chemical kinetics equations, uniquely define a special set of water quality equations. These are numerically integrated as the simulation proceeds in time. At user-specified print intervals, values of selected state variables are saved for subsequent evaluation in visualization and statistical post-processor programs.

Advective and dispersive transport fields are required for the transport sub-model. These will be specified using input from the hydrodynamic model, POM, with translation provided by USACOE-WES. Once specified, transport of temperature will be used to check the validity.

In addition to the loads for solids, settling and resuspension rates to and from bottom sediments must be specified. These will be estimated at fine scale using a sediment transport model, SEDZL (see above).

2. Data Quality - All target model analyte (mercury, PCB congeners, TNC, and atrazine) and most supporting analytical and in-field data were collected and analyzed in compliance with an USEPA approved QAPP. Louis Blume, GLNPO QA Manager, and a team of QC Coordinators with specific knowledge, hands-on experience and training in the analysis of the target analytes verified the data using a software package developed by Environment Canada. The program is called Research Data Management and Quality Control System (RDMQ) and runs on a SAS-based platform. The requirements for the data precision, accuracy, representativeness, comparability, completeness and sensitivity contained in each researcher's approved QAPP are programmed into RDMQ. When the requirements are not met, the data are flagged and brought to the attention of the QC Coordinator for resolution with the researcher. RDMQ also will allow for reconciliation of field collection and sample analysis information. The QC data reported by the researchers such as lab, trip and field blank contents, lab and field duplicate results, matrix and surrogate spike recoveries, reference material results and calibration check data are assessed during the RDMQ verification and the QC Coordinator determines if any noncompliant data affects the project data. An additional code is added to any affected data by the QC Coordinator if in their assessment the data are biased high, biased low, or invalid. No values are censored before release to the modelers, they are only flagged.

B. Model Development

1. Code Development and Maintenance - The basis for the water quality models will be "IPX-MT" (modified transport) which incorporates QUAL-ICM advective-dispersive transport with GBTOX organic carbon sorbent dynamics and IPX solids transport. These latter models were both versions of WASP4 developed during the Green Bay Mass Balance Study (GBMBS) Each of these models has been checked and documented (Velleux *et al*., 1993). The Lake Michigan mass balance models will use IPX-MT as the initial chassis. The code will be modified to include those processes included in GBTOX, a mass balance model developed and applied for Green Bay (Bierman *et al*., 1992; DePinto *et al*., 1993). Each chemical-specific model will contain a unique set of processes in addition to the normal transport and solids submodels.

   The code used in the mass balance water quality model is written in FORTRAN. Coding is done using standard programming practices and all code changes are rigorously checked and debugged. Development and production code is maintained at LLRS in the RCS.

2. Model Documentation - A complete description of the model equations, underlying assumptions, boundary conditions, and numerical methods are

contained in several user manuals for WASP (Di Toro *et al*., 1983; Ambrose *et al*., 1993) and QUAL-ICM (Cerco and Cole, 1995). The revised Lake Michigan mass balance models will be documented in a final report.

3. Code Verification - The modeler may make the code changes or may delegate this to a programmer. For either case, the modeler is ultimately responsible for the code changes and should double check all algorithms. The Digital UNIX FORTRAN compiler provides a variety of source code error checking, which is also invoked during model code development and testing.

   Water modeling codes are typically verified with tests against analytic solutions, against results from previous versions, and by sensitivity analyses. Verification of any code is achieved over the long run by distributing it to other users for application at other sites. Users are asked to notify LLRS of any bugs found. The ideal situation for code verification would be for independent programmers and modelers to thoroughly review the equations and codes. This may be achieved in part by the peer review process.

4. Code Documentation - Modelers and programmers continuously document their work within computer programs and in their project notebooks. Information in this documentation include a description of the change, date of change, and name of person making the change. As model computer programs are developed, user manuals will be prepared as the formal documentation.

5. Model Calibration/Verification and Uncertainty - The general validity of mass balance models can be judged according to their track record of simulating measured conditions and predicting future conditions. Several "post-audit" studies have been done for the eutrophication models (Di Toro *et al*., 1987; Bierman and Dolan, 1986) and one post-audit was conducted for the Saginaw Bay PCB model (Endicott and Kandt, 1994). A post-audit was performed by comparing predicted concentration to independent measurements. The post-audit studies, although not perfect, show a reasonable level of credibility for mathematical models.

   The Lake Michigan mass balance models will be calibrated by comparing computed concentration for appropriate spatial segments to appropriately averaged field data. The model will be considered calibrated when the calculated concentration representing spatially averages in time compare within one standard error of the data volume weighted average by cruise.

   Once comparable to field data, the model will be valid within the error constraints specified for the calibration period. However, the question of uncertainty remains for the predicted future concentration. For the predictions, the model will be run for various scenarios of inputs, boundary conditions, and process rates bracketed in terms of extreme expectations and probability distributions. The results will be provided in terms of prediction means and exceedence limits.

   Model results will also be qualified according to the any explicit and implied assumptions made in developing or applying the model. It is expected that the "science review panel" will also provide caveats for the model results. Managers will have to decide whether or not to use the model results and whether or not to conduct additional research to improve the models. This is a continuing process.

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Phytoplankton Solids/Eutrophication Model

Principal Investigators: William Richardson and Douglas Endicott, USEPA, LLRS
Contract Support Modeler: James Pauer, SoBran, Inc.

A. Model Description

1. Background Information - Modeling eutrophication and phytoplankton solids in lakes are a complex issue which can be approached on many levels. The extent and complexity of the modeling exercise depends on the time and manpower resources available, and the quality and quantity of the data. Historical eutrophication models range from simplistic empirical models, e.g., predicting phytoplankton chlorophyll as a function of the total phosphorus concentration (Dillon and Rigler, 1974) to "state-of-the-art", multi-class, multi-segmentation models with sophisticated kinetic and transport processes (Bierman and McIlroy, 1986; Cerco and Cole, 1995).

   Several models have been developed for the Great Lakes, including Lake Michigan and Green Bay. These are mass balance models (Lake-1, originally developed in the mid-70's by the Manhattan Group, Thomann *et al*., 1975 and applied to many Great Lakes Systems, Di Toro and Connolly, 1980; Rodgers and Salisbury,

1981) which fundamentally calculated concentrations of phytoplankton and zooplankton biomass as a function of lake nutrient levels. The MICH1 model (Rodgers and Salisbury, 1981) was developed specifically to describe eutrophication and phytoplankton production in Lake Michigan and was verified with an extensive water quality database from 1976-77 (which is now available in STORET). These models reflected the state of eutrophication theory at the time, and were published in the primary literature for review by the scientific community. In recent years, several advances have been made in eutrophication modeling such as variable phosphorus stoichiometry, internal nutrient pool kinetics, sophisticated sediment submodels, incorporation of multi-phyto- and zooplankton classes as well as zebra mussels. These improvements have been incorporated into models such as WASP5 (Ambrose *et al*., 1993), The Saginaw Bay Multi Class Model (Bierman and McIlroy, 1986), and CE-QUAL (Cerco and Cole, 1995) which has been applied to several systems, including the Great Lakes.

2. Model Equations, Systems, and Parameters - Modeling eutrophication involves estimating biomass (phyto- and zooplankton) as a function of nutrients which are present in the lake in different domains (water column and sediments), oxidation states, and forms (particulate or dissolved). The systems include diatoms, other algae, zooplankton, soluble reactive phosphate, particulate and dissolved organic phosphate, ammonium, nitrate, particulate and dissolved nitrogen, dissolved and biogenic silica. Equations have been formulated to describe the biochemical transformation reaction between the different systems. Phytoplankton production can be modeled based on traditional growth kinetics which is dependent on nutrient levels, light intensity, temperature, and water turbidity (Thomann *et al*., 1975; Chapra, 1997). The nutrient dependency is usually modeled according to Monod kinetics, a semi-empirical equation (Monod, 1942) applied to a multitude of lake and river eutrophication models over many decades (Thomann *et al*., 1975; Cerco and Cole, 1995). Predation and mineralization are described according to "commonly accepted" eutrophication theories (Di Toro and Connolly, 1980), which have stood the test of time.

   Since several equations are used to describe the nutrient/plankton interactions, a large number of model parameters have to be estimated, including rate coefficients for algal growth and death, predation by zooplankton, and mineralization of organic nitrogen and phosphorus. Coefficient values are also required to accommodate and describe temperature and light interactions, sediment diagenesis and transport such as settling and resuspension. A complete list of model parameters is too large to include here. These details are contained in the model and code documentation (Thomann *et al*., 1975; Di Toro and Connolly, 1980; Rodgers and Salisbury, 1981; Ambrose *et al*., 1993) as well as textbooks and other documents (Chapra, 1997; Thomann and Mueller, 1987; Bowie *et al*., 1985) as listed in the references below and are available for inspection at the LLRS.

3. Data Quality - Historical data are obtained from several sources, primarily STORET. STORET contains all of the GLNPO's historical data for Lake Michigan. Records extend back to 1961. The quality of this information is, to a large extent, unknown. However, all historical data will be screened for reasonableness before use. If questions arise, attempts will be made to contact the originating laboratory. The final model calibration and verification will be done using the 1994-95 project data which will pass through an intense QA/QC protocol. A limitation of the eutrophication modeling design is the limited number of specific laboratory and field studies done to estimate the large number of model coefficients. It is, therefore, necessary to depend on literature values for the different parameters. Coefficients will be obtained mainly from historical studies performed in Lake Michigan and the other Great Lakes. Care will be taken to selectively use coefficient values from credible sources such as NOAA, GLERL and University of Michigan. Further refinement of these coefficients will be done during the calibration process. This process will be

documented in detail in the accompanied report for the LMMBP modeling study.

B. Model Development

1. Code Development and Maintenance - The development of a eutrophication model for Lake Michigan will take place in phases. The first phase will begin by resurrecting historical eutrophication models for Lake Michigan and Green Bay, as described in the Background Section. These historical models were generally developed as tools to predict the phytoplankton standing crop (as chlorophyll *a*) and its impact on water quality in terms of transparency (aesthetics), dissolved oxygen, taste and odor. The shift of the emphasis of this modeling project is to estimate the autochthonous phytoplankton solids, expressed as organic carbon, which will be used in a sorbent dynamic model for hydrophobic toxic chemicals. Figure 5 shows a diagram of the dynamics of the phytoplankton and detrital carbon in the lake. In brief, the extent of growth of the phytoplankton and subsequent phytoplankton solids concentration is a function of the nutrient levels and is mediated by meteorological conditions, such as temperature and solar radiation, as well as water turbidity. In addition, it is affected by rates of settling of the phytoplankton species, higher predation by the zooplankton, and sediment-water interactions. Code modifications will be done to adapt the models to incorporate this shift of emphasis, as well as to be specifically used for modeling eutrophication in Lake Michigan.

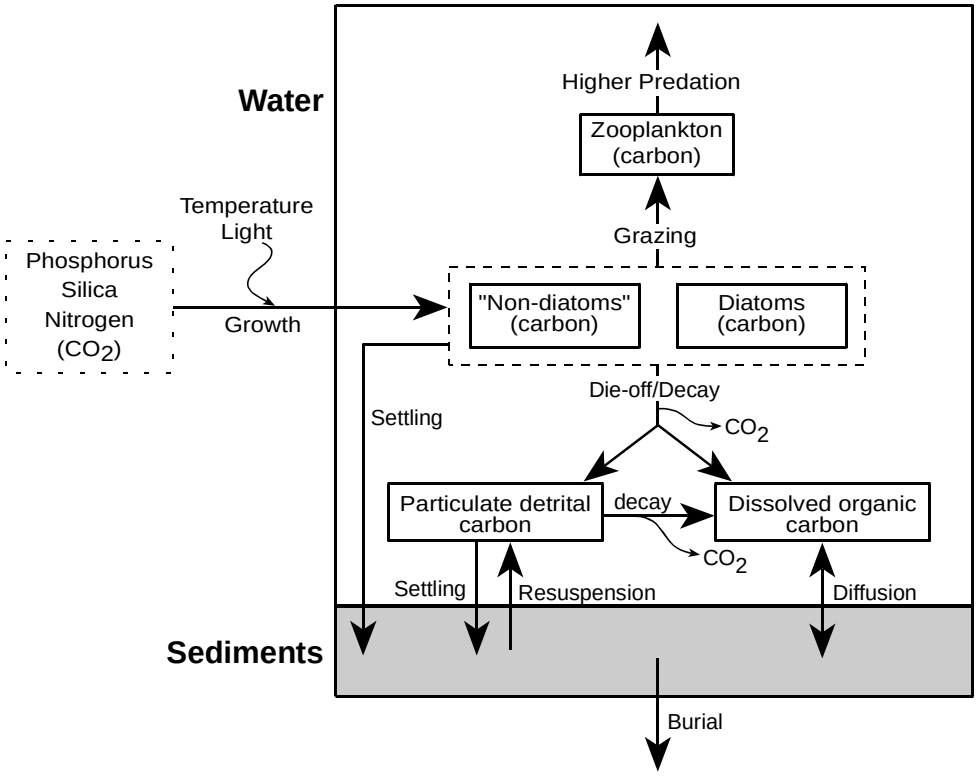

Figure 5. Phytoplankton and Detrital Carbon Dynamics in Lake Michigan.

The next phase will be the development of a model (or modification of an existing framework) which incorporate recent "state-of-the-art" eutrophication kinetics, transport and water-sediment interactions. Two frameworks are considered: the existing IPX framework originally developed at the USEPA LLRS for modeling toxic chemicals in the Fox River (Velleux *et al*, 1994), and the CE-QUAL-ICM framework developed by the USCOE (Cerco and Cole, 1995). Proposed features of the model will be including the simulation of multiple phyto- and zooplankton species, hydrodynamics on a small grid size and sediment-water interactions. Both models have a few limitations and further development and code modifications will be performed. The eutrophication model will be applied to both the 41 water column segmentation scheme (as used by some of the other models) and the ultimate higher order multi-segmentation grid. It is foreseen that the 41 segmentation model will be based on the CE-QUAL framework, while the IPX model will be used for the multi-segmentation model. Output from the two models will be compared, which will improve the credibility of both frameworks. Code development will be done using the RCS code management tool and all changes to the code will be documented as much as possible within the code, as well as in a subsequent report or paper. Specifics for any new model(s) or modifications will be incorporated into this QA plan as they are finalized.

2. Model Documentation - The calibrated, verified, and tested model(s) will be documented as a technical report and/or scientific paper. This will include the description of the basic assumptions, fundamental equations, and model coefficients. In addition, all changes/improvements to the model framework will be documented in detail.

3. Model Validation and Uncertainty Analysis - The models will be validated during (a) the development and testing period, as well as (b) verification of the final code using field (project) data.

   (a) The modifications to the models will be tested against the original equations. In addition, output from the modified models will be compared to the original or similar models.

   (b) The models will be calibrated using a field data set and adjustments will be made to the model to "fit-the-data". An independent data set (both sets probably using the 1994-95 project data) will be used to verify the model. Uncertainty analysis is an important issue when modeling eutrophication since there are so many degrees of freedom (independent coefficients that have to be estimated). A number of techniques are available to determine the sensitivity of these parameters on the overall model output, and the uncertainty and error involved (e.g., Monte Carlo analysis). A suitable technique(s) will be selected and used to evaluate the model.

C. References

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Atrazine Water Quality Model

Principal Modelers: Kenneth R. Rygwelski and William L. Richardson, USEPA, LLRS

A. Model Description

1. Background Information - As a precursor to atrazine models for the LMMBP, a screening-level WASP-based mass balance model (Endicott *et al*., 1992) was developed to gain an initial insight to the chemical's behavior in the basin. This screening model utilized historical data that pre-dates the LMMBP data set. The results of this screening-level model strongly suggest that atrazine is not degrading in the large, cold, oligotrophic waters of Lake Michigan, and this conclusion is similar to some other lakes reported in the literature. While volatilization, associated with solids, and kinetic degradation are probably active in this lake, their overall affect on transport and fate of atrazine is suspected to be minimal according to a literature review. Lake Michigan MICHTOX runs from 1964 to 1993 indicate that the lake is steadily increasing in atrazine concentration. Model results fall within a range of +/- one standard deviation about the mean of the field data from 1991 and 1992.

   Ongoing modeling efforts will address atrazine transport and fate in Lake Michigan utilizing all of the atrazine data associated with the LMMBP including atrazine degradation products, deisopropylatrazine and deethylatrazine. This high resolution model will include processes such as volatilization and, perhaps, association with solids. WASP-based models will be used.

2. Model Parameters - A generic description of the types of model parameters to be used by the Lake Michigan Project models was described in above and are applicable to the atrazine models. The screening-level atrazine model described above and a thorough literature search on atrazine processing in freshwater helped in the QA process by identifying parameters that are important to the model predictions. Tributary loadings of atrazine and the degradation products, deethylatrazine and deisopropylatrazine are very significant parameters to the model. Also, loadings in the form of wet precipitation (rain and snow) are important. Parameters associated with processes such as volatilization, association with solids, accumulation in biota, and kinetics *in-situ* degradation are of much less importance in model predictions, because they are likely to be minor processes.

   Model parameters that are unique to the atrazine model are watershed-type information: Watershed Export Percentage, hydrologic soil type; atrazine application rates to corn by county, by year in the basin; county size; fraction of county in the Lake Michigan basin; and corn acreage by county. Also, total annual atrazine usage in the United States is used to estimate historical loadings of atrazine in Lake Michigan.

3. Data Quality - Atrazine, and its metabolites deethylatrazine and deisopropylatrazine will be measured in the lake and tributaries by Eisenreich and Rutgers. Hites and Ilora of Indiana University and Sweet of Illinois State Water Survey will measure atrazine in the air vapor phase, wet precipitation, and dry particulate (air). Both total and dissolved forms will be measured. All of these data will be collected under USEPA QAPP, and will be QA-reviewed by Louis Blume of USEPA GLNPO with assistance from contractor staff. A QA-review data software package called RDMQ will assist in the QA review process according to requirements of the approved QAPP's associated with each parameter. RDMQ is owned by Environment Canada, Atmospheric Environment Service, Ontario, Canada. RDMQ runs under the SAS software system that allows: data visualization, corrects data (e.g., blanks, etc.), user-defined outlier checking, auditable trail of data changes, system-generated reports documenting the data quality flags, and handles checks on blanks, lab QC samples, matrix spike samples, duplicate samples, splits, composites, detection limit, etc. Only data that has passed GLNPO's data review process will be used in the atrazine model.

   Some of the data that will be used in the models will not be processed by RDMQ, because the data were collected prior to the Lake Michigan Project by other researchers. For instance, Watershed Export Percentages were obtained from peer-reviewed journal articles. Total annual United States atrazine usage was obtained from Arnold Aspelin, USEPA, Biological and Economics Analysis Division. Soil hydrologic types were obtained from William Battalin of USGS. Data on corn acreage, application rates of atrazine by county, and other agricultural data were obtained from Bruce Kirshner, IJC.

B. Model Development

1. Code Development and Maintenance - The code used in the atrazine model is based on the FORTRAN code of the WASP-IPX model as described by Velleux *et al*. 1994. The adaptation to Lake Michigan is based on both WASP-IPX and GBTOX used for the GBMBS (Bierman *et al*., 1992).and subsequent incorporation of QUAL-ICM advective-dispersive transport solution.

2. Model Documentation - The basic model equations, underlying assumptions, and numerical methods are documented in the WASP-IPX model documentation, the GBTOX report (Bierman *et al*., 1992), and the QUAL-ICM user's guide (Cerco and Cole, 1995). Modifications for the revision for Lake Michigan will be included in an updated documentation report. Interim documentation will be maintained within computer program code and the programmer's notebooks and electronic files.

3. Code Verification - See "General Considerations for All Mass Balance Water Quality Models" above.

4. Code Documentation - See "General Considerations for All Mass Balance Water Quality Models" above.

5. Model Calibration/Validation and Uncertainty - See "General Considerations for All Mass Balance Water Quality Models" above for information on this topic. Also, the following text highlights some other aspects of model calibration/validation for atrazine modeling in Lake Michigan.

   As mentioned earlier in this section, a screening level model of atrazine was developed for Lake Michigan based on historical data from the literature. This model helped identify a model approach and provided some insight into processes that may be important when the atrazine model based on Lake Michigan project data are used. The screening model identified tributary loadings and precipitation loadings as being the most important in terms of impacting lake concentrations. Within the tributary load estimates, one of the most important factors was the Watershed Export Percentage.

   Also, the screening model results suggest that kinetic decay, association with solids, and volatilization are not important in Lake Michigan, because the model was able to predict lake concentrations with export of mass associated with flows out as the only major operative loss mechanism. The processes that control most of the model output will also be those that will have the most effect on overall model uncertainty.

   Tributary loadings for 1995 will be estimated by both actual measurement of flows and concentrations of atrazine at the mouths of major tributaries leading to Lake Michigan. Also, tributary loadings to the lake will be estimated based on algorithms that utilize information such as total annual United States usage and Watershed Export Percentages. Comparing these two results helps verify loadings data.

   Three estimates of precipitation loadings should be available in the project: actual measured fluxes based on a sampling program; fluxes predicted by an air model component of the project; and estimates based on total annual usage. Data from all three of these estimates will be compared and help in the model validation process.

C. References

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Mercury Model

Principal Modeler: Kenneth R. Rygwelski, USEPA, LLRS

A. Model Description

1. Background Information - Ongoing modeling efforts will address mercury transport and fate in Lake Michigan utilizing all of the mercury data associated with the LMMBP. A literature review has been completed on mercury cycling in lakes, and as a result of this investigation, the Lake Michigan mercury model will likely include processes such as volatilization of Hg(0); tributary loads of Hg(2+) and methyl mercury; and atmospheric inputs of Hg(2+). Processes involving Hg(2+) and methyl mercury with biotic and abiotic solids will be important. The Hg(2+) and methyl mercury species form complexes with a number of anions that are present in the water, and those that are especially important in Lake Michigan are neutral complexes with the chloride and hydroxyl ions. The relative abundance of these inorganic anions is important in predicting the overall mix of the complexed mercury species. This prediction is accomplished using an equilibrium speciation model such as MINTEQA2 (ftp://ftp.epa.gov/epa.ceam/ wwwhtml/ minteq.htm). It is important to understand the composition of the mercury complexes in Lake Michigan because the overall observed chemical properties of mercury is dictated by this composition. For example, the overall octanol-water partition coefficient for Hg(2+) is strongly dependent on the actual complexes of Hg(2+) present in the lake. The octanol-water partition coefficient (K_{ow}) for $Hg(Cl)_2$ is 3.33, whereas the K_{ow} for $Hg(OH)_2$ is 0.05. Studies have shown that mercury uptake by diatoms is a function of the overall K_{ow} of the particular mercury species that is present. Higher overall K_{ow}'s result in higher uptake (Mason *et al*., 1996).

2. Model Parameters - A generic description of the types of model parameters to be used by the Lake Michigan Project models was described above and are applicable to the mercury models. In addition, data on the various forms of mercury Hg(2+), Hg(0), and methyl mercury will be needed. Chloride concentrations and pH of the lake water will also be required to assess complexation of the various mercury species.

3. Data Quality - Total and dissolved mercury will be measured in the lake and tributaries by Mason of University of Maryland and Hurley of University of Wisconsin, Water Chemistry Laboratory, respectively. Dr. Gerald Keeler of the University of Michigan will be providing data on mercury in precipitation (wet and dry) and vapor phase concentrations. Rossmann of USEPA LLRS, will be measuring mercury in sediments. All of these data were collected under USEPA QAPP and will be QA-reviewed by Louis Blume of USEPA GLNPO with assistance from contractor staff. A QA-review data software package called RDMQ will assist in the QA review process according to requirements of the approved QAPP's associated with each parameter. RDMQ is owned by Environment Canada, Atmospheric Environment Service, Ontario, Canada. RDMQ runs under the SAS software system that allows data visualization, corrects data (e.g., blanks, etc.), user-defined outlier checking, auditable trail of data changes, system-generated reports documenting the data quality flags, and handles checks on blanks, lab QC samples, matrix spike samples, duplicate samples, splits, composites, detection limit, etc. Only data that has passed GLNPO's data review process will be used in the mercury model.

B. Model Development

1. Code Development and Maintenance - The code used in the mercury model is based on the FORTRAN code of the WASP-IPX model as described in Velleux *et al*., 1994. The adaptations to Lake Michigan is based on both WASP-IPX, GBTOX used for the GBMBS (Bierman *et al*., 1992) and subsequent incorporation of QUAL-ICM advective-dispersive transport solution.

2. Model Documentation - The basic model equations, underlying assumptions, and numerical methods are documented in the WASP-IPX model documentation, the GBTOX report (Bierman *et al*., 1992) and the QUAL-ICM user's guide (Cerco and Cole, 1995). Modifications for the revision for Lake Michigan will be included in an updated documentation report. Interim documentation will be maintained within computer program code and the programmer's notebooks and electronic files.

3. Code Verification - See "General Considerations for All Mass Balance Water Quality Models" above.

4. Code Documentation - See "General Considerations for All Mass Balance Water Quality Models" above.

5. Model Calibration/Validation and Uncertainty - See "General Considerations for All Mass Balance Water Quality Models" above. Also, the following text highlights some other aspects of model calibration/validation for mercury modeling in Lake Michigan.

   In order to gain an initial insight to mercury cycling in Lake Michigan, a screening-level model will be developed. This screening model will include volatilization, association with solids, and mass gain due to precipitation and tributary loadings. Mass loss with flow out of Lake Michigan will also be included. This model will have low spatial and temporal resolution. MINTEQA2 will be used outside of the construct of the mass balance model to gain an understanding on the composition of the various mercury species complexes on a range of expected pH and chloride concentrations in the lake. Hopefully, this screening-level exercise will identify important factors controlling model predictions. Since very little mercury speciation was analyzed, assumptions on likely predominant species in the various model components will need to be made. In addition, the significance of methylation/demethylation reaction rates for mercury in water, suspended solids, and bed sediments must be evaluated.

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PCB/TNC Model

Principal Modeler: Douglas Endicott and William Richardson, USEPA, LLRS
Support Modeler: Xiaomi Zhang, SoBran, Inc.

A. Model Description

1. Background Information - PCBs have been the subject of considerable research since their discovery in the Great Lakes ecosystem in the early 1970's. The first models of toxic chemical transport and fate were developed for the Great Lakes by Thomann and Di Toro (1983). This framework was also applied to Saginaw Bay (Richardson *et al*., 1983) which was the first attempt to calibrate a model to a synoptically collected dataset for PCBs. A screening level model was developed for PCBs and other toxic

chemicals in Lake Michigan to provide insights on program design and research needs (Endicott *et al*., 1992). A major step in improving the PCB modeling framework was taken during the GBMBS. The basic WASP transport and fate framework was revised to include more detailed processes involving particulate fractions (Bierman *et al*. 1992, DePinto *et al*., 1993a). This model is referred to as GBTOX. In the same project, WASP4 was also modified to improve the simulation of sediment transport, based upon process research and modeling of settling and especially resuspension processes in the Fox River (Velleux *et al*., 1994). This model was named IPX. As described previously in this Plan, the transport and fate model for toxic chemicals in Lake Michigan will be based upon a combination of features taken from these models. Each of these models has been developed to simulate the transport and fate of PCBs, which serve as model chemicals for a class of semi-volatile, hydrophobic toxic chemicals which also includes TNC.

2. Model State Variables and Parameters - PCBs will be modeled as 34 individual congener peaks (half of which comprise two coeluting congeners). These congeners were selected based upon their detection across all or most media sampled; they are listed in Table 1. In a review of preliminary data from the Project, the 34 congener peak concentration sum was found to be greater than 50% of the total PCB concentration in air vapor, precipitation, lake water, suspended solids, sediment, phytoplankton, and lake trout. Therefore, we feel confident that model predictions of total PCB concentration can safely be extrapolated from the congener-specific results. The list of congeners selected for modeling may be revised, as necessary upon examination of the full database.

   Other than the PCB congener and TNC toxic chemical state variables, the model will also include three organic carbon sorbents: biotic carbon (BIC), particulate detrital carbon (PDC), and dissolved carbon (DOC). The autochthonous (internal) loading of BIC and DOC are derived from the eutrophication model simulation.

Table 1. PCB Congener Peaks Selected for Transport and Fate (Mass Balance) and Bioaccumulation Modeling.

IUPAC	Homolog	Comment
3	Mono	
6+5	di	
12+13	di	
15+17	di/tri	
16+32	tri	
18	tri	
26	tri	
31	tri	
33	tri	mono-ortho
37	tri	coplanar
44	tetra	
49	tetra	
52	tetra	
56+60	tetra	
66	tetra	
70+76	tetra	
74	tetra	
77+110	tetra/penta	coplanar
81	tetra	coplanar
84+92	penta	
99	penta	
101	penta	
118	penta	mono-ortho
123+149	penta/hexa	
132+153	hexa	mono-ortho
151	hexa	
163+138	hexa	
170+190	hepta	
172+197	hepta/octa	
180	hepta	
182+187	hepta	
195+208	octa/nona	
196+203	octa	
201	octa	

External loading of toxic chemicals, categorized as tributary loading, atmospheric wet deposition, and dry particle deposition, as well as external loading of organic carbon sorbents, will be estimated from the project data by the LMMBP Atmospheric Modeling and Loading Workgroups. Lake boundary and initial condition concentrations will be computed from project data, and will be verified by model calibration results. Atmospheric vapor-phase boundary conditions will be calculated by the Atmospheric Modeling Workgroup.

Transport parameterization includes specification of advective and dispersive water column transport, pore water diffusion, vertical particle transport, and sediment bioturbation. Advective and dispersive transport will be based upon results of hydrodynamic model simulations. This input will be confirmed using conservative tracer and temperature simulations. Particle transport parameters include settling and resuspension velocities. Particle-class specific settling velocities will be calculated from sediment trap data, while resuspension velocities will be based upon resuspension flux simulations from SEDZL. Sediment bioturbation will be calibrated to radionuclide profiles measured in sediment cores. Sediment core data will also provide particle burial rates, which will be used to confirm the rates of burial independently computed by the model as the difference between settling and resuspension.

Parameters used to describe the dynamics of the organic carbon sorbents include the rates and yield of organic carbon transformation between state variables (including temperature dependence) in both water column and sediment, the rates of organic carbon mineralization, and the diffusion rates for DOC within the sediment and at the sediment-water interface. A general strategy for calibration of these parameters was developed during the GBMBS (DePinto *et al*., 1993b). If possible, however, these parameters will be coupled to the corresponding parameters within the eutrophication model simulation.

Chemical-specific processes include partitioning between aqueous and organic carbon sorbents, and volatile exchange between the surface water and atmosphere. The model will describe chemical partitioning between dissolved and particulate sorbent compartments, including multiple particle types, using an organic carbon-based equilibrium assumption. Both local equilibrium and first-order kinetic partitioning process descriptions will be tested in the model. Upon the recommendation of the Atmospheric Modeling Group, the volatilization formulation described by Hornbuckle *et al*. (1995, 1997) will be applied. Forcing functions from the hydrodynamic model input will be used to compute local volatilization rates in the transport and fate model. Henry's constant for each chemical will be based upon literature review, and will be adjusted for surface water temperature. Chemical transformation by biotic or abiotic reactions, is assumed to be negligible for PCBs and TNC.

Rates will be specified initially from literature values and previous modeling studies. They may be adjusted during model calibration. The specific parameters and detailed description are contained in the references listed below.

3. Data Quality - The data used will extracted from the project database which will have been thoroughly checked as described in the general section above. Initial estimates for model parameters will be obtained from the literature as well as prior modeling applications. Parameter values adjusted during calibration must pass a test for reasonableness, including falling within a range of "probable" values.

B. Model Development

1. Code Development and Maintenance - IPX-MT is coded in ANSI standard FORTRAN 77, with subroutines and common variable blocks stored in separate source and include files. UNIX Makefile is maintained for program compilation. The FDCHAIN source code and all associated files are maintained using the Digital UNIX

RCS. Code modifications to the model will be done in-house at the LLRS.

2. Model Documentation - Model documentation is provided in a series of reports and publications cited above. A User's Guide, based upon Velleux and Endicott (1994), is maintained at LLRS. As the model program is revised and modified, updated documentation is added to the User's Guide.

3. Code Verification - Code changes are carefully done according to appropriate process information. Codes are checked and results will be compared to hand calculations. Modifications made to the model will be verified by first testing against results from the original version to ensure proper function of the code. Testing will then verify the performance of new or revised model features. Details of testing performed on model revisions will be recorded and retained within modeler notebooks.

4. Code Documentation - IPX-MT code has been internally documented, by its original developers and by programmers and modelers at LLRS. The history of revisions to the model code is maintained, both as chronological entries within the header comments of each file and within RCS. Details will also be retained within project modeler/programmer notebooks.

5. Model Calibration/Validation and Uncertainty - Comparison of observed and predicted chemical concentrations in water, suspended solids, and sediment serves as the basis for model calibration and confirmation. These comparisons will include two- and three-dimensional visualization of concentration predictions and residuals, as well as conventional calibration plots of predictions and residuals as functions of time and depth. Model goodness-of-fit will be evaluated for individual observations as well as for spatial averages of data comparable to model segmentation.

   The database and modeling design are constrained so that the primary chemical-specific process requiring parameter calibration is partitioning. Initial values of chemical-specific organic carbon partition coefficients (K_{oc}) will be based upon averages calculated from the data. At the same time, variation in K_{oc} due to explanatory variables such as season, depth, organic carbon source and composition, and disequilibria, will be evaluated. This information will guide refinement of partitioning parameters during model calibration.

   Once comparable to field data, the model will be valid within the error constraints specified. The question of uncertainty will remain for the predicted future concentrations. For the predictions the model will be run for various scenarios of inputs, boundary conditions, and process rates bracketed in terms of extreme expectations and probability distributions. The results will be provided in terms of confidence levels about the most probable.

   Model results will also be qualified as all models are simplifications of the real system and contain many explicit and implied assumptions. It is expected that the "science review panel" will also provide caveats for the model results and include recommendations for future work to reduce uncertainty. Managers will have to decide whether or not to use the model results and whether or not to conduct research to improve the models. This is a continuing process.

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Bioaccumulation and Ecosystem Models

Food-Chain Model for PCBs and TNC in Lake Michigan

Principal Modeler: Douglas Endicott, USEPA, LLRS
Support Modeler: Xin Zhang, PAI/SoBran, Inc.

A. Model Description

1. Background Information - The food web bioaccumulation model predicts chemical concentrations in biota in response to chemical concentrations in water and sediment. Bioaccumulation in Lake Michigan lake trout and coho salmon will be modeled using an age-class model for hydrophobic organic chemical bioaccumulation in aquatic food webs, FDCHAIN. The formulation of this model follows the developments of Nordstrom *et al*. (1976), Weininger (1978), Thomann and Connolly (1984), Thomann (1978) and Connolly *et al*. (1992). Food web bioaccumulation models have been successfully applied for PCBs and other hydrophobic organic carbon (HOCs) in several large-scale aquatic ecosystems including Lake Michigan (Thomann and Connolly, 1984), New Bedford Harbor (Connolly, 1991) and, most recently, for the GBMBS (Connolly *et al*.,1992). The model developed for that project, FDCHN, will be adapted for use in Lake Michigan.

   For Lake Michigan, bioaccumulation of PCB congeners and TNC will be modeled for lake trout and coho salmon food webs. Food web bioaccumulation will be simulated for sub-populations of lake trout in three distinct biotic zones. The general structure of the lake trout food web in Lake Michigan is shown in Figure 6.

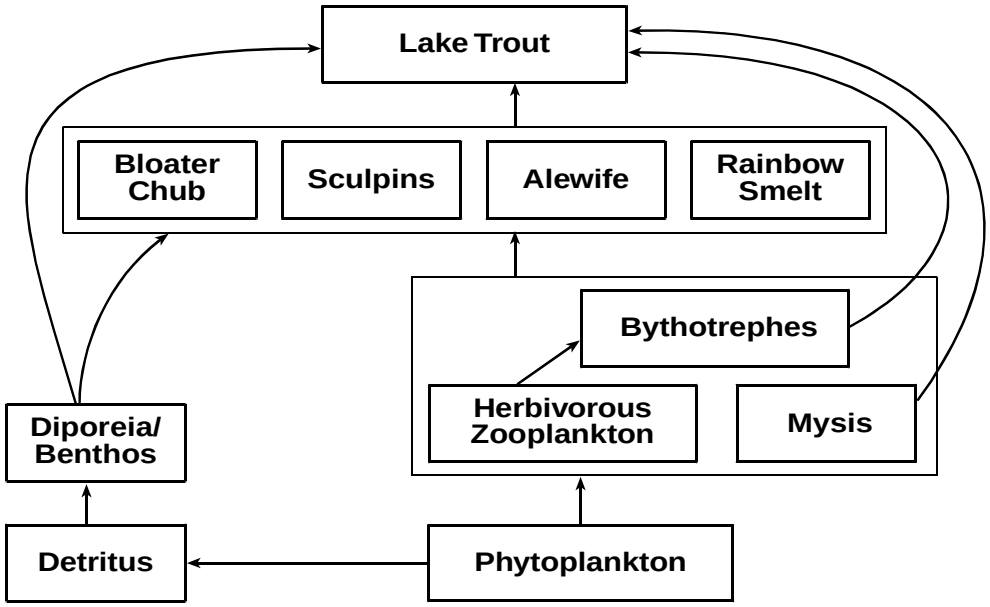

Figure 6. Lake Michigan Lake Trout Food Web Spatially and Temporally Variable: Age Dependent.

In each zone, different food webs support lake trout, including benthic and pelagic food web linkages. Biotic zones are defined by the approximately 50-mile range of movement of lake trout. The coho salmon, in comparison, is strictly pelagic. Although the coho food web is simpler, the bioaccumulation simulation must account for significant migration over the two year lifetime of this stocked salmonid in Lake Michigan.

2. Assumptions - FDCHN is a time-variable, population-based age class model, incorporating realistic descriptions of bioenergetic, trophodynamic, and toxicokinetic processes. The general features of FDCHN are well-suited to a modeling application such as the LMMBP. The general form of the bioaccumulation equation equates the rate of change in chemical concentration within a fish (or other aquatic organism) to the sum of chemical fluxes into and out of the animal. These fluxes include direct uptake of chemical from water, the flux of chemical into the animal through feeding, and the loss of chemical due to elimination (desorption and excretion) and dilution due to growth. To predict bioaccumulation for top predator fish (the modeling objective here), the bioaccumulation mass balance is repeatedly applied to animals at each trophic level to simulate chemical biomagnification from primary and secondary producers, through forage species to top predators. Chemical biotransformation (metabolism), an additional loss mechanism, is apparently negligible for most PCB congeners in fish, and will be neglected for this application. Other assumptions made by this model include:

   a. Only freely-dissolved chemical is bioavailable: Thus, particulate and colloidal (DOC) chemical phases are not available for uptake by biota, unless they are ingested.

   b. Lipids are the storage reservoir: Other tissues are only important in determining rates of chemical transfer within the organism. The model only accounts for

HOC accumulation in a single lipid compartment.

c. The BCF (bioaccumulation factor) and lipid-water partition coefficient are correlated to the octanol-water partition coefficient, K_{ow}. For HOCs up to about log K_{ow} of 6.0 to 6.5, they are approximately equal. Such a correlation is not apparent for chemicals with higher K_{ow} values. Why such "super-hydrophobic" chemicals do not follow the bioconcentration behavior of other HOCs has not been resolved. However, most of the abundant PCB congeners in Lake Michigan have log K_{ow} values less than 6.5, therefore this uncertainty is not a major problem.

3. Model Parameters - The data requirements to support a scientifically defensible, state-of-the-art food web bioaccumulation model are exhaustive. Yet, because the LMMBP was designed with a modeling objective, it supported many of these data requirements. These data have been categorized as follows:

   Biota (collection and analysis): The collection, characterization, and contaminant analyses of samples of all species selected to represent the Lake Michigan food web. Biota sampling was designed to capture the trends in chemical concentrations in fish and lower food web organisms, including variations due to age, spatial distribution, and season, for each species modeled in the food web. Food webs were sampled for sub-populations of lake trout in three distinct biotic zones. A lake-wide grid sampling design was required to sample coho salmon. Four collection seasons were established for fish: spring, summer, and fall of 1994, and spring of 1995. For each fish species, five replicate composite samples were formed and analyzed for fish collected in each zone and collection season. For lake trout and coho salmon, composites were formed according to age, while for forage species the composites were based upon size.

   To define suitable initial conditions for the model, and to allow model testing over longer than the two year duration of the mass balance project, historical biomonitoring data will be used. Total and Aroclor PCB concentrations have been monitored in Lake Michigan lake trout and coho salmon since 1972, by USEPA and the States. Several studies have confirmed the analytical comparability of the historical and mass balance data, at least for total PCB.

   Mysis and *Diporeia* were sampled in biota zones, as well as sediment sampling locations, using a benthic sled. Phytoplankton and zooplankton were sampled by filtration at the 41 water quality monitoring stations. Samples of suspended particulate matter passing a 100 micron nominal pore size glass fiber filters were operationally defined as phytoplankton, while those trapped by the filter were defined as zooplankton.

   Toxicokinetic parameters: The toxicokinetic parameters of the bioaccumulation model define the rates of chemical uptake from water, excretion from the organism, and transfer from the diet. In general, these parameters are a function of both the contaminant and the organism. Estimates of these parameters based upon laboratory data are quite variable, and establish only broad limits to guide model calibration. These parameters include the uptake rate from water, the excretion rate, and the chemical (dietary) assimilation efficiency.

   Bioenergetics: Biological attributes of each organism that affect bioaccumulation, including rates of growth (wet weight and lipid), consumption, and respiration. Bioenergetic data required for bioaccumulation modeling includes rates of growth (wet weight and lipid), consumption, and respiration for each species as a function of age or weight, temperature, season, and biota zones. For the Lake Michigan application, growth rates were based upon regression of age and weight data. The length, weight, and age of each fish collected during the project was determined, allowing direct estimation of seasonal growth rates for all species. The lipid content [g(lipid)/g(wet) body weight] was also determined for all fish collected in the project. Time functions of lipid content

were constructed for each species, incorporating both age-dependence and seasonal variation observed in the lipid data. The lipid time series were then input to the bioaccumulation model. Respiration rates were calculated from a standard allometric relationship, dependent on weight and temperature, which was fitted to laboratory data for each species. Species-specific data for SDA (specific dynamic action) were also included in the respiration rates.

Ecological characterization: Data defining the Lake Michigan ecosystem in terms of food web structure and species migration. Food web structure: Accurate characterization of the diet of each fish modeled in the food web is important, because chemical transfer associated with food ingestion is the primary route for hydrophobic chemical accumulation. Fish diets are determined by analyzing stomach (gut) contents, and this data is then generalized in terms of the fraction (by weight) of each prey species consumed. For lake trout and coho salmon, prey species and size were determined as a function of predator size and age. Spatial and seasonal variation in fish diets were also factored into the model parameterization of food web structure. These sources of information were used to construct food web structures for each biota zone.

Fish movement and migration: Migration may be defined as the movement of fish between habitats suitable for feeding, reproduction, and refuge in periods of unfavorable conditions. The movement between habitats is strongly influenced by the diel pattern of light and dark, the annual temperature and photoperiod cycles and the age and sex of the fish. In addition, the habitats suitable for feeding and refuge may be different depending upon life stage. The general migration patterns of individual fish species have been determined from tagging studies. These sources of information were used to define species-specific migration patterns for the model.

B. Model Development

1. Code Development and Maintenance - The FDCHAIN model follows the developments of Nordstrom *et al*. (1976), Weininger (1978), Thomann and Connolly (1984), Thomann (1978) and Connolly *et al*. (1992). Version 5.0 of FDCHN, developed by Manhattan College and HydroQual, Inc. (HydroQual, 1996) for the USEPA GBMBS, will be adapted for use in Lake Michigan. FDCHAIN is coded in ANSI standard FORTRAN 77, with subroutines and common variable blocks stored in separate source and include files. A UNIX Makefile is maintained for program compilation. The FDCHAIN source code and all associated files are maintained using the Digital UNIX RCS.

2. Model Documentation - Model documentation is provided in a series of reports and publications cited above. A User's Guide, based upon the 1996 HydroQual report, is maintained at LLRS. As FDCHAIN is revised and modified, updated documentation is added to the User's Guide.

3. Code Verification - FDCHAIN has been tested through it's application in a number of projects, as described above. Modifications made to FDCHAIN will be verified by first testing against results from the original version to ensure proper function of the code. Testing will then verify the performance of new or revised model features. This will consist of comparisons of intermediate and final model results to hand (or spreadsheet) calculations over several integration time steps. "Extreme case" scenarios will be selected for these tests, to amplify errors and maximize the likelihood of their detection.

4. Code Documentation - FDCHAIN code has been internally documented, by its original developers and by programmers and modelers at LLRS. The history of revisions to the FDCHAIN code is maintained, both as chronological entries within the header comments of each file and within RCS.

5. Model Calibration/Confirmation and Uncertainty - Comparison of observed and predicted species-

specific chemical concentrations serves as the basis for bioaccumulation model calibration and confirmation. Comparisons will include chemical concentration variation between age classes, across trophic levels, and between seasons and biota zones, as well as comparisons based upon standard data transformations such as bioaccumulation factors and predator-to-prey contaminant ratios. Toxicokinetic parameters, which are most often adjusted to calibrate the model, will be treated as constants, or varied according to hydrophobicity of the chemical and trophic level of the organism. Such a systematic approach to toxicokinetic parameterization will be sought, in order to reduce degrees of freedom in the calibration of the model.

Our experience with past food web bioaccumulation modeling projects, especially in the GBMBS, suggests that even with a good database for model calibration, large uncertainties in model predictions may result due to unexplained variability and overparameterization in the model. We propose to evaluate and estimate bioaccumulation model uncertainty using the Bayesian Monte Carlo (BMC) (Dilks *et al*., 1992) method. BMC generates estimates of model uncertainty that are unaffected by parameter covariance, a factor that causes traditional Monte Carlo analysis to significantly inflate model uncertainty.

It should be recognized that FDCHN, and in fact, all current food web bioaccumulation models, is not predictive in terms of the dynamics of the food web itself. In other words, the food web structure is described as model input. FDCHN does not predict changing forage composition, trophic status in response to nutrients, exotic species invasion, or fisheries management. Yet such factors have been demonstrated to alter food web structures in the Great Lakes, and these changes have been suggested to affect bioaccumulation in top predators including salmonids. To address the sensitivity of bioaccumulation predictions to food web dynamics, the SIMPLE model (Jones, *et al*., 1993), a bioenergetic model for fish population dynamics in the Great Lakes, will be used to construct scenarios for food web change that will then be tested in FDCHN. Such testing will demonstrate the sensitivity of bioaccumulation predictions to food web dynamics in comparison to changes in contaminant concentrations in fish due to reducing exposure concentrations.

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Ecosystem Model

Project Officers: Glenn Warren, USEPA, GLNPO; Russell Kreis, Jr., USEPA, LLRS
Principal Modeler: Victor J. Bierman, Jr., Limno-Tech, Inc.

A. Model Description

1. Background Information - This model will build upon and enhance the Phytoplankton Solids/Eutrophication Model (PSEM) in the LMMBP. Consistent with the approach used in the GBMBS (Bierman *et al*., 1992; DePinto *et al*., 1993), the contaminant transport and fate models in the LMMBP will include explicit representation of sorbent dynamics in terms of particulate and dissolved organic carbon. An important component in the mass balance cycle for organic carbon is internal loading due to autochthonous (phytoplankton) production. Consequently, the mass balance model for sorbent dynamics must also include a eutrophication model for generating internal organic carbon loadings due to primary production.

   The PSEM in the LMMBP will be based on historical eutrophication models for the Great Lakes and on recent "state-of-the-art" eutrophication kinetics, transport and water-sediment interactions. These models will be modified to explicitly represent particulate and dissolved organic carbon dynamics, and to be compatible with the sediment and contaminant transport and fate models in the LMMBP.

   A limitation of the PSEM is that it does not represent lower food web components important to the Lake Michigan ecosystem such as *Bythotrephes*, *Mysis*, and possibly, *Pontoporeia* and zebra mussels. Interactions among phytoplankton groups and these lower food chain components are important processes that can influence organic carbon sorbent dynamics and contaminant transport, fate and bioavailability. More broadly, contemporary questions posed by resource managers require consideration of ecosystem productivity, risk-based ecosystem responses and effects, and ecosystem sustainability. Conventional water quality/eutrophication models do not provide answers to these questions because they contain only very simplified representations of lower food webs; they do not represent upper trophic levels, and they do not represent linkages between lower food webs and upper trophic levels.

   To address these important questions a new generation of models is evolving which contain explicit representations of ecosystem structure and function. For example, Limno-Tech, Inc. (1995, 1997) has developed and applied a coupled primary productivity-exotic species model to investigate responses of multiple algal groups in Saginaw Bay to changes in external phosphorus inputs and zebra mussel densities. The original Chesapeake Bay Water Quality Model (Cerco and Cole, 1994) has been enhanced to include micro- and meso-zooplankton, three functional groups of submerged aquatic vegetation, epiphytes and two types of benthic organisms, a filter-feeder and a deposit-feeder.

   The Lake Michigan Ecosystem Model (LMEM) will be an enhanced version of the PSEM and will constitute the first step towards a

comprehensive Great Lakes Ecosystem Productivity Model that could be used to investigate ecosystem-level responses and effects. The LMEM will include enhancements to the phytoplankton-zooplankton kinetics, with specific representation of lower food web components important to the Lake Michigan ecosystem.

2. Model Equations, Systems and Parameters - The LMEM will be constructed using mass balance principles and it will be compatible with other models used for the LMMBP. The LMEM will build upon the original eutrophication models developed for Saginaw Bay (Bierman and Dolan, 1981, 1986a, 1986b; Bierman and McIlroy, 1986; Bierman *et al*., 1980) and will contain multiple nutrients, multiple algal groups, and herbivorous and carnivorous zooplankton. Additional enhancements will be included to represent lower food chain components important to the Lake Michigan ecosystem such as *Bythotrephes*, *Mysis*, and possibly, *Pontoporeia* and zebra mussels.

   The final equations, systems and parameters in the LMEM will be based on a literature review of the Lake Michigan ecosystem, with emphasis on the lower food web. Principal emphasis will be placed on primary productivity and interactions of primary producers with higher trophic levels. A preliminary bibliography of the Lake Michigan ecosystem has been assembled and is appended to this QA/QC plan. A literature review on contemporary water quality and aquatic ecosystem models will also be conducted.

3. Data Quality - The primary source for historical data will be the USEPA STORET database. STORET contains all of the field data collected for Lake Michigan by the USEPA GLNPO since 1961. Emphasis will be placed on intensive studies conducted in 1976-77 and 1982-83. Because the quality of this historical information is uncertain, all of the STORET data will be screened for reasonableness by USEPA or its contractors before they are used. Attempts will be made to contact the originating laboratory in the event that questions arise. Final model development and application will be conducted using the 1994-95 project data. These data will be subject to a comprehensive QA/QC protocol before they are used for the modeling effort.

   An obstacle to development, calibration and verification of the LMEM is that routine field monitoring studies were not designed to measure state variables or internal model coefficients in "state-of-the-art" eutrophication models or in the new generation of evolving ecosystem models. Consequently, it will necessary to use data sets of opportunity acquired during the many specialized studies of Lake Michigan and other Great Lakes. It will also be necessary to depend on the published scientific literature for model conceptual development and for many of the internal model coefficients.

   Appropriate care will be taken to use datasets from reliable sources and to depend on personal communications with investigators who have a long history of experience in conducting studies on Lake Michigan and other Great Lakes. All data sources will be documented in detail and periodic review will be made to the QA/QC plan for the LMEM.

B. Model Development

1. Code Development and Maintenance - Code development and maintenance for the LMEM will be a collaborative effort between Limno-Tech, Inc. and USEPA LLRS. A detailed plan for model coding can not be developed until the conceptual framework for the LMEM is finalized. Code development and maintenance for the LMEM is expected to parallel these same tasks for the PSEM.

   At the present time there are two possible coding frameworks for both the PSEM and the LMEM: first, the WASP/IPX framework originally developed for modeling toxic chemicals in the Fox River (Velleux *et al*., 1994); and second, the CE-QUAL-ICM framework developed for modeling eutrophication in Chesapeake Bay (Cerco and Cole, 1995). There are also two

spatial segmentation grids for the LMMBP: first, a 41 water column segment grid; and second, an ultimate higher order grid that will represent Lake Michigan at either a 5 km or 10 km spatial scale. The coding framework(s) for these two models will depend, in part, on the spatial segmentation grid(s) to which each model will be applied.

Code development will be conducted using the RCS code management tool and all changes to the computer code will be documented to the fullest extent possible within the code itself, as well as in a subsequent technical report. As appropriate, periodic revisions will be made to the QA/QC plan for the LMEM.

2. Model Documentation - The development and application of the LMEM will be documented in the form of a technical report and/or scientific paper for the peer-reviewed literature. Documentation will include a description of the model conceptual framework, model assumptions, model state variables and process mechanisms, governing equations and tables of all model inputs and internal model coefficients. Numerical values will be presented for all model inputs and coefficients, along with sources from which these values were obtained.

3. Model Validation and Uncertainty Analysis - A detailed plan for model validation and uncertainty analyses can not be developed until the conceptual framework for the LMEM is finalized. In general, it is expected that validation and uncertainty analyses for the LMEM will parallel these same tasks for the PSEM. The QA/QC plan for the LMEM will be revised in the future to include specific plans for these tasks.

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Load Computations Models and Estimation Methodologies

Terrestrial Emissions and Atmospheric Fate and Transport Estimates for Atrazine and Mercury

Principal Investigator: Ellen Cooter and Russell Bullock, NOAA

This modeling component addresses the emissions of agricultural use of atrazine from the soil, the emission of mercury via an emissions inventory, development of a database of driving meteorological conditions and the estimation of fate and transport of atrazine and mercury from the eastern two-thirds of the United States and Canada to the surface of Lake Michigan. Three models and an emissions inventory are required for this task.

Emissions of Agricultural Use of Atrazine from Soil (ORTECH Soil Emissions Model)

Principal Investigator: M. Tevor Scholtz, ORTECH Corporation

A. Model Development

1. Background Information

Development History - The occurrence of pesticides and other persistent organic pollutants in areas of the globe which are being used, is of growing concern. The effects of several pesticides on animals and birds have been observed and documented. The effects of pesticides in the environment on humans are less clear but, nonetheless, there is a growing consensus that releases to the environment must be minimized or even eliminated for some pesticides.

In order to address these concerns regarding persistent organic pollutants (POPs), the United Nations Economic Commission for Europe (UNECE) has initiated the development of a protocol on POPs with Canada as the lead country. A task force has been formed which will assess the possible effects of POPs in the environment and will investigate strategies to eliminate POPs which are shown to have the potential to induce adverse responses in humans and in the environment. Participating countries have been requested to submit production and consumption as well as emissions inventory data for a selection of priority POPs. Included in the list are a number of pesticides, some of which are in current use in Canada while others have been banned or severely restricted.

The presence of pesticides in the Arctic and upper Great Lakes indicates that the atmospheric route is important and, in some cases, the dominant pathway for the translocation of pesticides following their application to agricultural lands. Deposition to the Great Lakes is thought to have significant contributions from local sources as well as long-range transport over regional and even global scales. The persistence of significant air concentrations of certain pesticides, the use of which has been discontinued in North America for some years, suggest that global transport is occurring from other parts of the world where such pesticides are still in use. Source/receptor relationships are extremely complex where such a wide range of distance scales is involved. Regional and global models are, therefore, being used to investigate such inter-relationships and to aid in the interpretation of the sparse measurements which are available. Emissions of pesticides to the atmosphere are critical inputs required by these models. Presently, there is no reliable way to estimate the emission of pesticides to air which result from their agricultural use. This model is the culmination of some six years of research which has involved developing, testing, and implementing a modeling capability for estimating the emissions of pesticides from vegetation and soils.

Application History - Development of a North American Pesticide Emission Inventory - At the current stage of the work, the potential for emission of twenty pesticides has been estimated; fourteen of these pesticides are on a combined Canadian and European nations priority list while the remaining six are heavily used in Canada. Pesticides are applied to agricultural crops and soils to control insects, weeds, and fungi which would otherwise reduce the productivity of cultivated land. Application may be as a spray or a dust, or pesticide may be incorporated into the soil at the time of planting of seed or tilling of the soil. Depending on the mode of application, some fraction of the applied pesticide is eventually emitted to the atmosphere from the soil surface and vegetation. Once in the atmosphere, transport, chemical transformation, and deposition of the pesticide to land and water surfaces will occur. Persistent organics which are deposited may also be re-emitted and in this way transported over global scales. The emissions model developed in this study is suitable for estimating emissions on time scales ranging from hourly to monthly, seasonal, or annual periods. The model comprises a one-dimensional numerical solution of the advection

and diffusion of heat, moisture and pesticide in agricultural soils with or without a crop cover. A simple canopy model has been developed to simulate the volatilization of pesticide from the vegetation. The model is driven by hourly meteorological observations which are available from North American climate stations. A series of experiments and sensitivity tests have been made with the model in order to gain insight into the post-application movement and emission of pesticides. These tests show that episodic emissions of pesticide due to tilling of the soil should not be overlooked. Tilling is an especially important emission source for persistent pesticides used on treated seed; tilling of the soil in the year subsequent to the planting of treated seed exposes pesticide residues to the atmosphere resulting in episodes of high emission during the tilling season. The emissions model is designed to run multi-year simulations of pesticide emissions with annual tilling so that pesticide residues are represented in the emission factors. Details of the theoretical development and testing of the pesticide emissions model and its application to the preparation of a North American pesticide emissions inventory are provided in the report.

The pesticide emissions model has been used to generate gridded emission factors for twenty selected pesticides including those on the international priority lists. The grid used covers the whole of North America but emissions from Mexico are not included in the inventory. The grid projection is polarstereographic with a grid size of 127 x 127 km; this grid is used by several of the Canadian regional transport and deposition models. The emissions over a two-year period have been simulated using 1989 meteorology obtained from approximately 80 climatic stations. Other inputs required by the model are gridded soil texture and properties, and the methods by which the pesticides are applied. Modeled seasonal and annual emission factors for the twenty pesticides studied are provided in the report on the 127 km grid. For the nine pesticides which were still being used in North America in 1989-1990, gridded seasonal and annual emissions are reported. Environment Canada (Yi-Fan Li, personal communication, 1995) provided the pesticide usage data required to compute emissions using modeled emission factors. The computed emissions include those due to pesticide residues remaining from the previous year's application.

As part of the Canada's involvement in the United Nations International Global Atmospheric Chemistry Program (IGAC), the CGEIC is presently completing a global pesticide emission inventory under the cooperative Global Emissions Inventory Activities working group (GEIA) which is a sub-program of IGAC. The methodology being used for this global study is similar to that described in the present report.

Planned Refinements - The model will be modified by Trevor Scholtz and associates at the CGEIC to incorporate grid-specific information and to enable it to make episodic emission estimates on a gridded basis. A report documenting the model changes will be produced.

2. Model Parameters

Soil parameters:

- Class
- Texture
- Field capacity
- Saturation capacity
- Permanent wilt point
- Saturation hydraulic conductivity
- Soil constant saturation matric potential

Geophysical, Climatological, and Crop Parameters:

- Last frost date
- Canopy shading factor
- Surface roughness
- Root development

Canopy Parameters

- Cuticle scale
- Droplet diameter

A.I. concentration
Pesticide application rate
Diffusivity in water
Diffusivity in cuticle
Air-side coefficient
Contact angle on cuticle
Friction velocity

3. Data Quality

Soil Texture - The original model used the UNEP/GRID (1992) two-minute latitude/longitude global grid of soil classes which was used to generate a FAO Soil Map of the World. The values were regridded to the CGEIC 127 x 127 km grid. For the LMMBP, the U.S. Department of Agricultural (USDA) Natural Resource Conservation Service State Soil Geographic Database (STATSGO) are used. Information regarding this database is found at: http:// www.agnic.nal.usda.gov/agdb/ statsgo.html. This original database has been modified to a 1 km spatial scale by scientists at PSU. The 1 km soil texture will be aggregated to the 36 km scale through area weighting. These values will be used to drive both the mesoscale meteorological model as well as the soil emission model.

Meteorology - Output from the modified PSU/NCAR mesoscale meteorological model version 5 (MM5-PX) will be supplied for each 36 km grid for each model hour over the study domain. Meteorological inputs to the soil emission model are as follows:

u wind velocity component
v wind velocity component
mixing ratio
pressure
precipitation
net radiation
deep soil temperature
Monin-Obukhov length
emissivity

Physical-Chemical Properties of Atrazine:

diffusivity in air (Sherwood *et al*., 1975)
diffusivity in water (Sherwood *et al*., 1975)
soil sorption (Wauchope *et al*., 1992)
solubility (Sunito *et al*., 1988)
Henry's Law constant (Sunito *et al*., 1988)
half-life in soil (Wauchope *et al*., 1992; Howard, 1991)

Pesticide Application Rate:

Estimated annual total atrazine applied per county acre representing 1995 is obtained from the USCG National Water Quality Assessment Pesticide National Synthesis Project. Documentation for this database, including sources and limitations is found at http://water.wr.usgs.gov/pnsp/use92/ mapex.htlml.

These data are regridded to the 36 km mesoscale modeling grid and reported as a total application (kg per year) for each grid cell.

Mode of Application and Number (Timing) of Application:

Assumptions reported in Scholtz *et al*. (1997) will be used unless additional information is obtained indicating other values are more appropriate.

Application Timing:

Atrazine is most often applied either as a pre-emergent or post-emergent spray. Emergence is assumed to take place seven days after planting. State level crop progress information is available from the USDA National Agricultural Statistical Service. Data and documentation may be found at http://www.mannlib.cornell.edu/reports/nassr/ field/per-bb. Post-emergent application is assumed to take place 28 days after planting. Label instructions should be made after the plant reached 38 cm and so only one pre-emergent and one post-emergent application is assumed in the United States. Scientists with the CGEIC will

decide on the most appropriate application mode for Canada.

B. Model Development

1. Code Development and Documentation

Solid Model Development - In this phase of the work, the soil model was developed to simulate the volatilization of pesticide from bare soil to which pesticides had been applied for agricultural purposes. In addition to meteorological data, the model required geophysical data and the soil and pesticide properties to be specified. Once the model had been coded, it was subjected to a series of sensitivity tests to gain an understanding of those model parameters which had the greatest influence on the model results. During this phase, the numerical model was also tested against an analytical solution of the equations to ensure that the code was giving realistic results under the restricted conditions for which an analytical solution is available.

Development of a Model of Volatilization from a Vegetation Canopy - The canopy model which has been developed is a simple mass transfer resistance model similar to the big leaf dry deposition models. The detailed mechanisms whereby pesticides are partitioned between plant material and the air, and subsequently transported to the atmosphere, or washed off into the soil, are not well understood. While some data are available on the rate of loss of pesticide applied to vegetation, these data are generally single measurements without the accompanying meteorological data needed to develop and test a model. In formulating the canopy volatilization model, every effort has been made to include the expected physical processes while keeping the model relatively simple to be consistent with current understanding of canopy volatilization processes. In addition to the partitioning properties of the pesticide, parameters such as the spray droplet size, wetting properties of the carrier liquid and growth state of the canopy are important and these parameters have been included in the model. The modeling of more complex processes which undoubtedly play a role within the plant tissue was not attempted.

Integration of the Soil and Canopy Models for Emissions - For the preparation of a pesticide emission inventory, it is necessary to integrate the numerical soil and canopy models over an extended period of simulations and to accumulate the total emission to the atmosphere. Given the amount of pesticide applied per unit area and the accumulated loss per unit area, an emission factor can be calculated. For pesticides which are highly mobile in the soil and which volatilize readily from the surface, the period of model integration required to capture the total loss from the soil may be quite short. For these pesticides, the soil concentration falls to an insignificant level at the end of the integration period due to loss by volatilization and/or leaching into the water table. Persistent pesticides, on the other hand, generally have low mobility in the soil and as a result, while emission rates may be relatively low, emission continues for an extended period which may cover several years for highly persistent insecticides such as DDT or lindane. Integrating the pesticide emissions model for an entire year requires considerable computer time. At present, some of the parameters needed as input to the model, such as pesticide degradation rate and modes of application, are poorly known. As new data become available for some of these parameters, it will be necessary to re-run the entire model. Since the objective of this part of the study was to estimate emission factors for as many as 100 pesticides, this would be an onerous task. To avoid the need to re-run the model in order to change certain parameters, an alternative methodology was developed, based on the linear properties of the model equations. This methodology permits emission factors to be pre-computed using standard model solutions and subsequently combined according to application scenarios and decay rate. Using this methodology, changes in model parameters such as mode of application and degradation rate can be factored into the solutions without the need to re-run the model for every scenario.

Full model code and code documentation reside at the CGEIC. For information, contact:

Dr. M. Trevor Scholtz
Manager, Environmental Computing and Modeling and Director, Canadian Global Emissions Interpretation Centre (CGEIC)
ORTECH Corporation
2395 Speakman Drive
Mississauga, Ontario, Canada L5K 1B3
Telephone: (905) 822-4111, Ext. 524
Fax: (905) 823-1446
E-mail: tscholtz@ortech.on.ca

2. Model Documentation - The principle source of model documentation is in the report by Scholtz *et al*. (1997).

3. Model Verification - Comparison of model results to results obtained from an analytical solution verified the computer code and showed that the numerical scheme, under the condition where a comparison with the analytical solution was possible, accurately simulated the solute advection and diffusion in the soil.

   An assessment of the major influences on the diurnal pattern of pesticide emission concluded that the major factor influencing short term variations in volatilization rate was the water flux. Variations in the aerodynamic resistance, which are diurnally variable, were shown to be of secondary importance.

   Pesticide residues in the soil which persist beyond the year of application can contribute significantly to emission in subsequent years. In the computation of total emissions in a particular year, it will be necessary to consider more than one year's application for persistent pesticides.

   Comparison of pesticides volatilization model results with field measurements from bare soil has shown that the proposed air-surface exchange model is able to predict hourly volatilization rates of spray-applied triallate and trifluralin, which are in reasonable agreement with field measurements.

   Comparisons between heat and moisture flux measurements and the results obtained from the heat and moisture transport modules of the model show that these are also in reasonable agreement, given that no soil temperature or moisture profile data were available with which to initialize the model.

   Further model runs are needed to examine the negative volatilization fluxes that have been observed.

   Concerning model sensitivity analysis, it is difficult to rank the sensitivity of the model to the various parameters tested since the sensitivity is, to some extent, dependent on the specific pesticide. Parameters to which the model seems to be insensitive are the application rate, the water film resistance and the diffusivity in the cuticle (or cuticle resistance). The effects of precipitation are large, as would be expected. Many of the modeled half-lives are in excess of 30-days while the observed data show relatively short half-lives in some cases. The model does not include pesticide dislodgement or degradation and these processes could contribute significantly to pesticide loss, leading to the relatively short half-lives observed in the field in some cases. Atrazine has a reported soil half-life of 60 to 90 days and so this model characteristic should not impact our LMMBP application significantly. The controlling resistance for transport from the leaf surface to the atmosphere appears from the model to be the air-side resistance.

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Mercury Emissions Inventory

All inventory of anthropogenic sources of atmospheric mercury has been developed and described in USEPA's Mercury Study Report to Congress as mandated in Section 112(n)(1)(B) of the Clean Air Act, as amended in 1990. This inventory accounts for a variety of industrial, commercial and residential source types within all 50 states of the United States. It has been subjected to rigorous peer review both inside and outside of USEPA and has been judged to accurately describe the total mass and spatial distribution of mercury emitted to the atmosphere from anthropogenic sources in the United States. This emission inventory has been used to support regional-scale atmospheric mercury deposition modeling, the results of which are also described in USEPA's Mercury Study Report to Congress. This regional scale modeling showed that, in addition to total mass, the chemical and physical forms of mercury emissions are important in determining the patterns and intensity of mercury deposition to the surface. Studies of the chemical and physical forms of mercury emissions from various source types are currently ongoing.

Atmospheric mercury emissions from natural sources and from anthropogenically contaminated soils and water bodies are not as well understood as are the current direct anthropogenic emissions to air. It can be reasonably assumed that these natural and recycled emissions are mostly in the form of elemental mercury gas due to the relatively high vapor pressure of elemental mercury versus its oxidized compounds. However, the total mass of natural and recycled mercury emissions and the spatial distribution of those emissions are not confidently known at this time. It may be possible to model natural and recycled mercury in the form of a global-scale background concentration if it can be determined that no such emissions are significantly concentrated near Lake Michigan.

Anthropogenic emissions of mercury from sources in Canada are currently being surveyed by Canadian federal and provincial governments and preliminary inventories from this effort are now available. An accurate emission inventory for Canada including chemical and physical form definitions will be required for an accurate modeling assessment of total mercury deposition to Lake Michigan.

Emissions of mercury from anthropogenic sources in Mexico and more distant countries might be adequately accounted for by the global-scale background concentration also used to account for natural and recycled emissions. It is generally thought that oxidized mercury emissions will mostly deposit to the surface or convert to the elemental form within the transport distance from Mexico to Lake Michigan. Atmospheric mixing of the remaining mercury from these distant anthropogenic sources could make their mercury plumes indistinguishable from global-scale emissions. We currently do not have a complete understanding of the global-scale transport of atmospheric mercury. Thus, the concept of a nearly constant global background concentration of elemental mercury gas may be invalid. However, in the absence of comprehensive emission inventories for all industrial nations and global-scale atmospheric models to use them, we are forced to employ

some form of background concentration or constant boundary influx concentration in our modeling of atmospheric mercury deposition to Lake Michigan.

Generation of Driving Meteorological Conditions (MM5-PX)

A. Model Description

1. Background Information - Development history (http://laurel.mmm.ucar.edu/mm5/overview.html). The PSU/NCAR mesoscale model is a limited-area, hydrostatic or nonhydrostatic, sigma-coordinate model designed to simulate or predict mesoscale and regional scale atmospheric circulation. It has been developed at PSU and NCAR as a community mesoscale model and is continuously being improved by contributions from users at several universities and government laboratories.

   The Fifth-Generation NCAR/PSU Mesoscale Model (MM5) is the latest in a series that was developed from a mesoscale model used by Anthes at PSU in the early '70's that was later documented by Anthes and Warner (1978). Since that time, it has undergone many changes designed to broaden its usage. These include (i) a multiple-nest capability, (ii) nonhydrostatic dynamics, and (iii) a four-dimensional data-assimilation capability as well as more physics options.

   The model (known as MM5) is supported by several auxiliary programs, which are referred to collectively as the MM5 modeling system. A schematic diagram (Figure 7) is provided to facilitate discussion of the complete modeling system. It is intended to show the order of the programs and the flow of the data and to briefly describe their primary functions.

   Terrestrial and isobaric meteorological data are horizontally interpolated (programs TERRAIN and DATAGRID) from a latitude-longitude mesh to a variable high-resolution domain on either a Mercator, Lamber conformal, or polar stereographic projection. Since the interpolation does not provide mesoscale detail, the

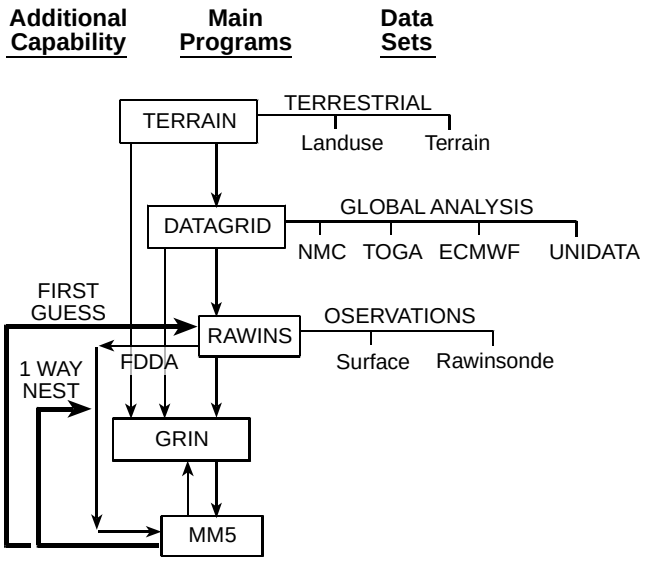

Figure 7. MM5 Modeling System.

   interpolated data may be enhanced (program RAWINS) with observations from the standard network of surface and rawinsonde stations using a successive-scan Cressman technique. Program INTERP performs the vertical interpolation from pressure levels to the sigma coordinate system of MM5. Sigma surfaces near the ground closely follow the terrain, and the higher-level sigma surfaces tend to approximate isobaric surfaces. Since the vertical and horizontal resolution and domain size are variable, the modeling package programs employ parameterized dimensions requiring a variable amount of core memory. Some peripheral storage devices are also used.

   MM5 model applications (http://laurel.mmm.ucjar.edu/mm5/application.html). MM5 has been used for a broad spectrum of theoretical and real-time studies, including applications of both predictive simulation and four-dimensional data assimilation to monsoons, hurricanes, and cyclones. On the smaller meso-beta and meso-gamma scales (2-200 km), MM5 has been used

for studies involving mesoscale convective systems, fronts, land-sea breezes, mountain-valley circulations, and urban heat islands. The model allows for multiple levels of nesting for cases involving scale interaction. A list of selected refereed journal publications related to PSU/NCAR mesoscale model version 5 is provided below.

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Planned Changes/Refinements - A number of shortcomings have been noted in the original MM5 approach to modeling the planetary boundary layer. Most particularly, the treatment of soil/vegetation interactions and convection phenomenon that are critical to the long-range fate and transport of atmospheric pollutants such as ozone. In response, a modified planetary boundary layer scheme was developed and is described in Pleim and Chang (1992) and Pleim and Xiu (1995).

A critical consideration when attempting to link models, with an eventual goal of coupling, is comparability of the underlying model physics. The original MM5 planetary boundary layer treatment is incompatible with the ORTECH soil emissions model physics. The MM5-PX physics are sufficiently similar that they can be considered comparable and the proposed model linkage for atrazine should yield results very close to that of a fully coupled.

2. Model parameters and how they will be specified (http://laurel.mmm.ucar.edu/tutorial-v2-notes.html) - Although the MM5 contains many fundamental physical relationships, parameterizations must still be used. Often there

are several parameterization choices for each process. The most critical parameterized processes and options are described below.

Cumulus parameterizations - none - uses no cumulus parameterization at grid sizes < 5-10 km.

Anthes-Kuo - based on moisture convergence, mostly applicable to larger grid sizes > 30 km. Tends to produce much convective rainfall, less resolved-scale precipitation, specified heating profile, moistening dependent upon relative humidity.

Grell - based on rate of destabilization or quasi-equilibrium, simple single-cloud scheme with updraft and downdraft fluxes and compensating motion determining heating/moistening profile. Useful for smaller grid sizes 10-30 km, tends to allow more resolved scale rainfall than convective rainfall.

Aradkawa-Schubert - multi-cloud scheme that is otherwise like Grell scheme. Based on a cloud population, allowing for entrainment into updrafts and allows for downdrafts. Suitable for larger scales, > 30 km grid sizes, possibly expensive compared to other schemes.

Fritsch-Chappell - based on relaxation to a profile due to updraft, downdraft and subsidence region properties. The convective mass flux remains 50% of available buoyant energy in the relaxation time. Fixed entrainment rate. Suitable for 20-30 km scales due to single-cloud assumption and local subsidence. See Fritsch and Chappell (1980) and Kain and Fritsch (1993) for details.

Kain-Fritsch - similar to Fritsch-Chappell, but uses a sophisticated cloud-mixing scheme to determine entrainment/detrainment, and removing all available buoyant energy in the relaxation time. See Kain and Fritsch (1993) for details.

Betts-Miller - based on relaxation adjustment to a reference post-convective thermodynamic profile over a given period. This scheme is suitable for > 30 km, but may not be suitable for severe convection. See Betts (1986), Betts and Miller (1986), and Betts and Miller (1993) for details.

PBL Schemes - none - no surface layer, unrealistic in real-data simulations.

Bulk PBL - suitable for coarse vertical resolution in boundary layer, e.g., > 250 m vertical grid sizes. Two stability regimes.

High-Resolution Blackadar PBL - suitable for high-resolution PBL, e.g., five layers in lowest km, surface layer < 100 m thick. Four stability regimes, including free convective mixed layer.

Burk-Thompson PBL - suitable for coarse and high-resolution PBL. Predicts turbulent kinetic energy for use in vertical mixing, based on Mellor-Yamada formulas.

Explicit Moisture Scheme - dry, no moisture prediction. Zero water vapor.

Stable Precip - nonconvective precipitation. Large scale saturation removed and rained out immediately. No rain evaporation or explicit cloud prediction.

Warm Rain - cloud and rain water fields predicted explicitly with microphysical processes. No ice phase processes.

Simple Ice (Dudhia) - adds ice phase processes to above without adding memory. No supercooled water and immediate melting of snow below freezing level.

Mixed-Phase (Reisner) - adds supercooled water to above and allows for slow melting of snow. Memory added for cloud ice and snow. No graupel or riming processes.

Goddard Microphysics - includes additional equations for prediction of ice number concentration and graupel. Suitable for cloud-

resolving models. See Tao *et al*. (1989, 1993) for details.

Reisner Graupel - based on mixed-phase scheme but adding graupel and ice number concentration prediction equations. Also suitable for cloud-resolving models.

Radiation Schemes - none - no mean tendency applied to atmospheric temperature, unrealistic in long-term simulations.

Simple Cooling - atmospheric cooling rate depends just on temperature. No cloud interaction or diurnal cycle.

Surface Radiation - this is used with the above two options. It provides diurnally varying shortwave and longwave flux at the surface for use in the ground energy budget. These fluxes are calculated based on atmospheric column-integrated water vapor and low/middle/high cloud fraction estimated from relative humidity.

Cloud-Radiation Scheme - sophisticated enough to account for longwave and shortwave interactions with explicit cloud and clear-air. As well as atmospheric temperature tendencies, this provides surface radiation fluxes. May be expensive but little memory requirement.

CCM2 Radiation Scheme - multiple spectral bands in shortwave and longwave, but cloud treated simply based on RH. Suitable for larger grid scales, and probably more accurate for long time integrations. Also provides -0 radiative fluxes at surface.

Ground Temperature Schemes - none - no ground temperature prediction. Fixed surface temperature, not realistic.

Force/Restore (Blackadar) Scheme - single slab and fixed-temperature substrate. Slab temperature based on energy budget and depth assumed to represent depth of diurnal temperature variation (-10-20 cm).

5-Layer Soil Model - temperature predicted in 1,2,4,8,16 cm layers (approximately) with fixed substrate below using vertical diffusion equation. Thermal inertia same as force/restore scheme, but vertically resolves diurnal temperature variation allowing for more rapid response of surface temperature.

3. Data Quality - Data obtained outside of LMMBP. (http://laurel.mmm.ucar.edu/mm5/tutorial-v2-notes .html). A great deal of input information is needed to set up a prognostic simulation. Three program modules focus on the input and modification of these data are described below.

   TERRAIN - The program that begins any complete forecast simulation is TERRAIN. This program horizontally interpolates (or analyzes) the latitude-longitude interval terrain elevation and land use categories onto the chosen mesoscale domains. The model domain settings (except for moving nests) are constructed in TERRAIN program. Users may use this program to check the correctness of the domain settings first without generating terrain height and land-use files. Once the domains are correctly set, users can then go on to run the program TERRAIN again to produce the terrain height and land-use files, which will be used by DATAGRID later.

   DATAGRID - The purpose of DATAGRID is to access archived low-resolution meteorological analyses:

   - Latitude-longitude grids
   - NMC: Global Analyses (1.5ox 2.5o).
   - ECMWF: Global Grids (2.5ox 2.5o; 1980-1989 only).
   - TOGA: Basic Level III data sets (2.5ox 2.5o).
   - Unidata: NMCMRF forecasts (2.5ox 5.0o).

   Horizontally interpolate these analyses to the model grid. Write the interpolated analyses for input to program RAWINS. The fields created by DATAGRID are used:

- To create model input fields directly from the DATAGRID output.
- As first-guess fields for subsequent objective analysis (program RAWINS).

Nonhydrostatic model input (or output) fields are:

3-D Field Name	Field ID (8 Characters)	Unit
U wind	U	kPa m/s
V wind	V	kPa m/s
Vertical wind	W	kPa m/s
Pressure perturbations	PP	kPa pa
Mixing ratio	Q	kPa kg/kg
Coriolis parameter	COROLIS	1/s
Map-scale factor	MAPFACCR	dimensionless
Map-scale factor	MAPFACDT	dimensionless
latitude	LATITCRS	degree
longitude	LONGICRS	degree
latitude	LATITDOT	degree
longitude	LONGIDOT	degree
Ground temperature	GROUNDT	K
Terrain elevation	TERRAIN	m
Land use	LAND USE	categories
Snow cover	SNOWCOVER	dimensionless

RAWINS - The purpose of RAWINS is to improve meteorological analyses (the first guess) on the mesoscale grid by objective analysis of surface and upper-air observations. The analyses input to RAWINS as the first-guess are generally the low-resolution analyses output from program DATAGRID. RAWINS may also use a MM5 forecast as the first guess.

RAWINS capabilities include:

- Choice of Cressman-style or Multiquadric objective analysis.
- Various tests to screen the data for suspect observations.
- Procedures to input bogus data.
- Expanded Grid - if you used an expanded grid in TERRAIN and DATAGRID, RAWINS can incorporate data from outside your grid to improve analyses near the boundaries. RAWINS cuts down the expanded grid to the unexpanded dimensions on output.
- Additional levels: RAWINS can interpolate from mandatory pressure levels to additional levels you specify for an analysis with higher vertical resolution.

RAWINS output is used to:

- Provide fields for initial and boundary conditions.
- Provide three-dimensional fields for analysis-nudging and four-dimensional data assimilation.
- Provide surface fields for surface-analysis nudging and four-dimensional data assimilation.

Source of Observations - NMC operation global surface and upper-air observations subsets as archived by the data support section at NCAR.

- upper-air data: ROBS, in MNC ON29 format.
- surface data: M.C. surface ADP data, in M.C. ON29 format.
- real-time (or recent) surface and upper-air observations from Unidata, in NetCDF format.

B. Model Development

1. Code Development/Maintenance and Documentation - The PSU/NCAR MM5 Source Code Documentation NCAR/TN-392+STR, by Philip Haagenson, Jimmy Dudhia, David Stauffer, and Georg Grell.

2. Model Documentation - (http://laurel.mmm.ncar.edu/mm5/doc.html). The MM5 is a community research model. It is open for access and modification by any research scientist. Documentation for the downloadable version is available as listed below. The full set has been broken into files whose sizes are listed in parentheses. All told, the full document is on the order of 100 pages. It should be noted that since the model is designed primarily for research applications, modification and development will continue. These files may be found at WWW site:

   A description of the Fifth-Generation PSU/NCAR MM5 includes:

   - Cover page (22928 bytes)
   - Table of Contents, Preface, and Acknowledgments (45613 bytes)
   - Chapter 1: Introduction and Chapter 2: Governing Equations and Numerical Algorithms (176803 bytes)
   - Chapter 3: The Mesh-Refinement Scheme (72278 bytes)
   - Chapter 4: Four-Dimensional Data Assimilation (200171 bytes)
   - Chapter 5: Physical Parameterizations (463327 bytes)
   - Appendices (173606 bytes)
   - References (51604 bytes)

   Due to the ongoing nature of the research and development, documentation may not be up-to-date or complete. Following is a list of available MM5 modeling system documentation as of July 1997. Among them, the PSU/NCAR Mesoscale Modeling System Tutorial Class Notes' is updated most frequently. These on-line MM5 documents are broken up into a number of smaller postscript files (the sizes of the files appear as part of the title). If you use the gopher or Mosaic browser to download the files, they may have a different file size. Users can download and print the documents at their site. Documentation is also available from NCAR's anonymous ftp site: ftp://ftp.ucar.edu/mesouser//Documents. When downloading from the anonymous ftp site, just get the *.tar.Z file.

   To order the hardcopy MM5 documents, send e-mail to Milli Butterworth (butterwo@ncar.ucar.edu) of UCAR Information Support Services. The fee for the documentation is $10.00 per document (includes shipping and handling).

   - Terrain and Land Use for the Fifth-Generation PSU/NCAR MM5: Program

     TERRAIN NCAR/TN-397+IA, by Yong-Run Guo and Sue Chen.

   - Data Ingest and Objective Analysis for the PSU/NCAR Modeling System: Programs DATAGRID and RAWINS NCAR/TN-376+IA by Kevin Manning and Philip Haagenson.

   - A Description of the Fifth-Generation PSU/NCAR MM5 NCAR/TN-398+STR, by Georg Grell, Jimmy Dudhia, and David Stauffer.

   - The PSU/NCAR MM5 Source Code Documentation NCAR/TN-392+STR, by Philip Haagenson, Jimmy Dudhia, David Stauffer, and Georg Grell.

   - PSU/NCAR Mesoscale Modeling System Tutorial Class Notes by Sue Chen, Jimmy Dudhia, Dave Gill, Yong-Run Guo, Kevin Manning, Dave Stauffer, and Wei Wang.

   - PSU/NCAR Mesoscale Modeling System Tutorial Class Notes (MM5 Modeling System Version 2) by Jimmy Dudhia, Dave Gill, Yong-Run Guo, Dan Hansen, Kevin Manning, and Wei Wang, February 1997.

- PSU/NCAR Mesoscale Modeling System Tutorial Class Notes (MM5 Modeling System Person 2) by Jimmy Dudhia, Dave Gill, Yong-Run Guo, Dan Hansen, Kevin Manning, and Wei Wang, July 1997.

3. Model Validation and Uncertainty Analysis - (http: //www.mcs.anl.gov/Projects/autodiff/weather/mm5.html). Sensitivity Analysis of a Mesoscale Weather Model, Christian Bischof, Gordon D. Pusch, and Ralf Knoesel.

   MM5, which was developed jointly by PSU Meteorology Department and NCAR, is a 3-D primitive-equation mesoscale weather model. Sensitivity analysis techniques are employed in atmospheric modeling, e.g., to develop a measure of reliability of a forecast or to assess to what extent a linearization of the model predicts the overall model behavior.

   To validate the sensitivity-enhanced MM5 code generated by ADIFOR, we can use automatic differentiation (AD) to produce a Tangent Linear Model (TLM) from MM5 by applying first-order perturbation theory. We then compare the sensitivities predicted by the TLM to divided-difference estimates obtained by running MM5 with small but finite perturbations about the base state.

   Work continues on a sensitivity-enhanced version of the Massively Parallel Mesoscale Model MPMM, a code developed here at Argonne under an internal grant, with additional support from the U.S. Air Force and the USEPA. The sensitivity-enhanced MPMM will make studies of much more complex problems practical, including treatment of nested subdomains. For more information, contact Gordon Pusch at <pusch@mcs.anl.gov> or Chris Bischof <bischof@mcs.anl.gov>. Argonne National Laboratory/Mathematics and Computer Science Division/autodiff@mcs.anl.gov.

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CMAQ

When concern over air quality developed in the United States and Canada several decades ago, the problem appeared to consist essentially of excessive local concentrations of common pollutants such as sulfur dioxide, particulates, carbon monoxide, and ozone. Air quality is now recognized as a much more complex problem or group of problems that span many pollutants having media-specific behaviors over very large geographic areas.

The role of atmospheric transport and deposition to the Great Lakes basin has been addressed under several modeling constructs, including mass balance models. In principle, the complex movements of pollutants through different parts of the environment can be described through a mass balance model. In practice, however, the data requirements needed to make reasonable estimates of the many processes involved are large, and sufficient data for these calculations usually are not available. Uncertainties are substantial even with the best available data on atmospheric and non-atmospheric inputs. The LMMBP study will seek to reduce uncertainty in the atmospheric component of the mass balance by employing mathematical models of atmospheric transport and deposition, to provide estimates for spatial and temporal gaps in actual monitoring databases and to test hypotheses about characterizations of atmospheric transformations and removal.

Air Quality Simulation Models (AQSMs) are frequently used to characterize the emission, transport, and deposition of hazardous air pollutants over large geographic areas. These models incorporate fairly extensive source emission inventories and meteorological databases (e.g., wind fields, temperature, mixing height), and apply the collected data to simulated processes such as dispersion, transformation, and deposition. The models are run to generate estimates of pollutant concentrations and deposition rates over a spatial and temporal pattern.

The mathematical relationships between emissions and concentration (or deposition) are typically nonlinear, due to the influences of the atmospheric transport, chemical and physical transformations, and deposition processes. Therefore, one cannot extrapolate, based on measurements alone, the quantitative relationship between changes in emissions and changes in atmospheric concentrations (or deposition). AQSMs attempt to account for the nonlinear physical and chemical processes influencing atmospheric concentrations deposition.

Development of AQSMs started in the late seventies. The Urban Airshed Model (UAM; Scheffe and Morris, 1993) followed by the Regional Oxidant Model (ROM; Lamb, 1983) provided Eulerian-based models for ozone, the former for urban and the latter for regional scale. Strategies for State Implementation Plans (SIPS) used ROM to provide boundary conditions for UAM simulations. Attention to acid deposition issues was addressed in the eighties with the development and evaluation of regional acid deposition models such as the Regional Acid Deposition Model (RADM; Chang *et al*., 1987), the Acid Deposition and Oxidant Model (ADOM; Venkatram *et al*., 1988) and the Sulfur Transport and Emissions Model (STEM; Carmichael *et al*., 1986). Other major modeling systems included the Regional Lagrangian Modeling of Air Pollution model (RELMAP; Eder *et al*., 1986), a Lagrangian framework system, and semi-empirical and statistical models. Models of this period were designed to address specific air pollution issues, such as ozone or acid deposition. Thus, flexibility to deal with other issues such as particulate matter or toxics was very limited. With the passage of the CAAA-90, a wide range of additional issues was identified including visibility, and fine and coarse particles, as well as indirect exposure to toxic pollutants such as heavy metals, semi-volatile organic species, and nutrient deposition to water bodies.

In the nineties, the USEPA embarked upon the development of an advanced modeling framework to meet the challenge posed by the CAAA-90. The Models-3 framework has been designed for holistic environmental modeling utilizing state of science representation of atmospheric processes in a high performance computing environment. Descriptions of Models-3 can be found in Novak *et al*. (1988) and Byun *et al*. (1998). The science components in Models-3 are called the Community Multi-scale Air Quality (CMAQ) system and are described briefly in Ching *et al*. (1998).

The Models-3/CMAQ system is designed as a multi-pollutant, multi-scale Eulerian framework air quality and atmospheric deposition modeling system. It contains state-of-science parameterizations of atmospheric processes affecting transport, transformations and deposition of such pollutants as ozone, particulate matter, airborne toxics, and acidic and nutrient pollutant species. It is this new modeling system that will be further enhanced and applied to address the specific areas of concern for the LMMBP study.

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Tributary Loading

Principal Investigator: David Hall, USGS
Project Officer: Glenn Warren, USEPA, GLNPO

Because the preparation of this section was delayed, it is being included as Appendix G. The entire document provided by the USGS is entitled, "Quality Systems and Implementation Plan (QSIP)" and can be obtained from David Hall, USGS, Middleton, Wisconsin.

PCB Tributary Loading Models

Project Liaison: Dale Patterson, WDNR
Principal Modeler: Mark Velleux, WDNR
Support Modeler: Jim Ruppel, WDNR

A. Model Description(s)

1. Background Information - Ongoing PCB transport and fate model development for three Wisconsin tributaries to Lake Michigan will provide estimates of present and future PCB export to Lake Michigan. The three tributaries to be modeled are: 1) the lower Fox River; 2) the Sheboygan River; and 3) the Milwaukee River/Cedar Creek. All three tributary models

will be based on the IPX framework development as part of the GBMBS effort (Velleux *et al*., 1996). Additional information on the background of IPX model framework is provided in the section on the PCB/TNC model for Lake Michigan.

2. Model State Variables and Parameters - PCBs will be simulated as one state variable, total PCBs; solids will also be simulated as one, two, or three state variables, depending on the range of physical characteristics observed for particles in each tributary. Total PCBs will be computed as congener and/or Aroclor sums. If data exist to define initial conditions and external loads, mercury and TNC may also be simulated for the lower Fox River.

   External loading of PCBs and solids from tributary watersheds will be estimated using the results of independent rainfall-runoff models and field verification data collected as part of priority watershed project and other non-point source pollution characterization efforts. In the lower Fox River, there are 19 point sources; total suspended solids (TSS) loads from these dischargers are monitored daily; PCB loads are assumed to be as monitored during the 1989 GBMBS. There are no significant TSS or PCB dischargers in the spatial domain of the Sheboygan or Milwaukee River.

   Initial PCB concentrations and other river bed sediment characteristics will be estimated from spatial analysis of sediment core samples and results of sediment probing. Boundary conditions will be estimated from mass balance study data as well as from archival data sources such as the USEPA STORET database.

   Transport parameters specified include advective and dispersive water column transport and particle transport. Advective transport will be based on flow measurements. Dispersive transport will be estimated from theoretical principles and confirmed through calibration of a conservative tracer (chloride) where data exist. In the lower Fox River, advective and dispersive pore water transport is also included and is estimated from the results of a regional groundwater transport model. Particle transport parameters include settling and resuspension. Particle settling velocities will be estimated from grain size data and calibration. Resuspension velocities will be estimated from the results of SEDZL-based sediment transport estimates and calibration. Sediment core data will be used to independently confirm predicted burial rates which are computed in the model as the difference between settling and resuspension fluxes.

   Particle and contaminant physicochemical parameters specified include the ratio of organic carbon to solids, water column and sediment DOC, sediment bulk density, volatile exchange between the surface water and atmosphere, and partitioning between dissolved and particulate carbon sorbent compartments. Equilibrium partitioning is assumed. Chemical transformations by biotic or abiotic reactions are assumed to be negligible.

3. Data Quality - The data used will be extracted from the project database, other data collection efforts for each tributary, and archival sources such as STORET. Other data collection efforts include: 1) the GBMBS; 2) Sheboygan River Remedial Investigation/Feasibility Study (RI/FS) and food chain study; and 3) the Milwaukee River Mass Balance Study. However, the completeness and quality of data for each tributary differs widely. These differences will affect the accuracy of model results.

   The lower Fox River has been studied extensively. In addition to the LMMBP and GBMBS, a series of extensive follow-up efforts to characterize PCB distributions in the water, sediments, and fish have been completed. These studies provide extensive data sets specifically tailored for model development. The completeness and quality of these data will permit development of a research quality model.

   The Milwaukee River has also been well studied, although less so than the lower Fox River. In addition to the LMMBP, the Milwaukee River

Mass Balance Study provides information to support model development. However, PCB sources as well as distributions in the river sediments are less well known. These factors will limit the accuracy of model development to the screening-level.

The Sheboygan River is less well studied. Although listed on the USEPA National Priority List of Superfund Sites in May, 1986, only a portion of the PCB-impacted areas of the river have been studied; estimates of PCB distributions in river sediments are highly uncertain. With the exception of data collected as part of the LMMBP, few water column PCB data exist to support model development. These factors will limit the accuracy of model development to the screening-level.

All assumptions and simplifications needed to develop each tributary model will be identified and discussed in the final report.

B. Model Development

1. Code Development and Maintenance - IPX is coded in ANSI standard FORTRAN 77, with subroutines and common variable blocks stored in separate source and include files. A UNIX Makefile is maintained for program compilation. Model source code and all associated files will be maintained in a limited access file space; as model development proceeds, Digital UNIX RCS will be used for code maintenance. Code modifications will be done in-house at WDNR with assistance from LLRS.

2. Model Documentation - Model documentation is provided in a series of reports and publications cited above. A User's Guide, based on Velleux *et al*. (1994) is maintained by WDNR and LLRS. As the model program is revised and modified, updated documentation is added to the User's Guide. Documentation efforts will be coordinated with LLRS for consistency.

3. Code Verification - Code modifications will be carefully implemented and tested to verify proper model performance. Modifications to the code will be checked with an appropriate number of hand calculations and verified by testing against results from the original version to ensure proper function of the code. Code verification efforts will be coordinated with LLRS for consistency.

4. Code Documentation - The IPX code has been internally documented. The history of revisions ot the code is maintained as chronological entries within the header comments of each file. Documentation of future revisions will also be included within RCS. Code verification efforts will be coordinated with LLRS for consistency.

5. Model Calibration/Validation and Uncertainty - Comparison to observed and predicted chemical concentrations in water, suspended solids, and sediment serves as the basis for model calibration and validation. These comparisons define model goodness-of-fit and include time series and point-in-time analysis of predictions and residuals. Calibrated model predictions of PCB and TSS export to Lake Michigan will be compared to export values estimated by the USGS using alternative methods. Additional information on the model calibration and verification is provided in the section on the PCB/TNC model for Lake Michigan.

   Quantitative uncertain analysis of model results for the lower Fox River model will be completed using the uncertainty analysis methodology developed for the Fox River/Green Bay models as part of the 1989 GBMBS (Di Toro and Parkerton, 1993). Uncertainty analysis of model results for the Sheboygan River and Milwaukee River screening-level models will be qualitative but will draw from the more rigorous analysis for the lower Fox River.

   Model results will be qualified as all models are simplifications of natural systems and contain many explicit and implicit assumptions. It is also expected that the LMMBP Science Review Panel will provide caveats for the model results and include recommendations for future research to reduce model uncertainty. Managers will need to decide whether or not to use model results and

whether or not to conduct research to improve these models.

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Atmospheric Loading for Mercury

Principal Investigator: Gerald J. Keeler, University of Michigan
Project Officer: Angela Bandemehr, USEPA, GLNPO

A. Project Planning and Organization

1. Introduction - This project to calculate total atmospheric mercury deposition estimates to Lake Michigan is in support of the larger LMMBP. The USEPA has adapted the mass balance approach to provide a consistent framework for integrating load estimates, ambient monitoring data, process research, and modeling to develop a predictive tool to guide future toxic load reduction efforts for Lake Michigan. The USEPA will coordinate the development of a suite of integrated mass balance models to simulate the transport, fate, and bioaccumulation of toxic chemicals in Lake Michigan. The four main goals of the LMMBP are to:

   a. Determine loading rates for critical pollutants from major source categories (tributaries, atmospheric deposition, contaminated sediments) to establish a baseline loading estimate to gauge future progress, and to better target future load reduction estimates.

   b. Predict the environmental benefits (in terms of reducing concentrations) of specific load reduction alternatives for toxic substances, including the time required to realize the benefits.

   c. Evaluate the environmental benefits of load reductions for toxic substances expected under existing statutes and regulations and, thereby, determine if there is a need for more stringent, future regulations to realize further benefits.

   d. Improve our understanding of how key environmental processes govern the transport, fate, and bioavailability of toxic substances in the ecosystem.

   The LMMBP model will initially use observation-based interpolation of atmospheric monitoring data, collected as part of the Enhanced Monitoring Program, to estimate atmospheric loading. The UMAQL collected samples for particulate phase mercury, vapor phase mercury, and mercury in precipitation from five sampling sites around Lake Michigan during the Lake Michigan Loading Study (July 1, 1994 through October 31, 1995). The UMAQL will utilize this monitoring data in a multi-tiered comprehensive approach to estimate both wet and dry atmospheric deposition estimates and associated uncertainties.

2. Background - Mercury is a toxic bioaccumulative substance in aquatic ecosystems. In its methylated form, mercury has been observed to bio-concentrate more than a million fold in the aquatic food chain. Consumption advisories are presently in effect for fish caught in Lake Michigan, Lake Superior, Michigan inland lakes, and a number of Wisconsin inland lakes because

of elevated mercury concentrations. Atmospheric deposition is widely recognized as an important link in the cycling of mercury in the environment and has been identified as the primary pathway for inputs of mercury to Lake Michigan. Consequently, mercury has been identified as a critical pollutant for study and has specifically been targeted in the 1987 GLWQA and Section 112(m) of the CAAA-90.

The GLWQA states that it is the goal of the Governments of Canada and the United States to restore and maintain the chemical, physical and biological integrity of the waters of the Great Lakes Basin Ecosystems. Further, these Governments have agreed to make a maximum effort to develop programs, practices and technology necessary for a better understanding of the Great Lakes Basin Ecosystem. As part of this effort, Annex 2 of the GLWQA mandates the development of LaMPs for each of the five Great Lakes, in an effort to address these issues on a lake-by-lake basis. A variety of activities, mandated by the GLWQA and the CAAA-90, including the LMMBP, are being performed in an effort to provide the information necessary to carry out the LaMP developed for Lake Michigan.

3. Project Objectives - The overall objective of this project is to obtain estimates of total mercury loading to Lake Michigan due to atmospheric deposition. These estimates will be based on data collected as part of the Enhanced Monitoring Program, including simultaneous measurements of mercury in air and water during lake-wide mass balance surveys, and during the intensive work sponsored by the USEPA.

   The specific objectives of this project are as follows:

   1. Determine that portion of the atmospheric deposition loading of total mercury to Lake Michigan due to "wet deposition". Estimates of the uncertainties associated with this calculation will also be addressed.

   2. Determine that portion of the atmospheric deposition loading of total mercury to Lake Michigan due to "dry deposition". To achieve this latter objective, two sub-objectives will also need to be addressed. Namely, this project will need to develop methods for:

      (a) the determination of dry deposition velocities and mercury volatilization rates, and

      (b) the determination of the vapor-phase concentrations for mercury in the air-water interface.

   Estimates of the uncertainties associated with this calculation will also be addressed.

4. Project Description - Meeting the project objectives described in Section I will require the utilization of newly developed wet- and dry-deposition estimation techniques that incorporate databases not previously used in atmospheric deposition calculations. The uncertainties in making over-water estimations with little meteorological or chemical data available are inherently large. Recent innovations in radar technology and advances in computer hardware have enabled scientists to begin developing new numerical methods of open water meteorological parameterization. The technical approaches and techniques used to achieve each of these objectives are discussed in detail below. A summary table of the methods to be used in these analyses is given at the end of Task 1.

   Task 1: Determine that portion of the atmospheric deposition loading of total mercury to Lake Michigan due to "wet deposition".

   Wet-deposition loading estimates will be calculated using a 5 km grid scale resolution for total mercury. A multi-level approach will be used to calculate the loading to Lake Michigan due to wet-deposition.

   Level One estimates are straightforward and will employ a modification of the method used by

Voldner and Alvo (1993). In this method, estimates of the total wet deposition to each grid cell within the 5 km grid domain will be derived from available monitoring site data using a spatial interpolation technique called kriging. First, monthly volume-weighted precipitation concentrations will be calculated for each LMMBP sampling site. These concentration values will then be interpolated across Lake Michigan using the aforementioned "kriging" technique, to obtain an estimate of "average concentration" for each grid cell. Similarly, monthly precipitation totals obtained from each of the NWS rain gauge network sites (approximately 700) will be "kriged" to obtain precipitation totals for each 5 km grid cell. The final wet deposition estimate would result from taking the product of the "kriged" concentration and precipitation fields. Uncertainties in this method will be based on uncertainties in the measurement and analysis of the samples, plus the uncertainties due to the interpolation technique (which are dependent on the location of the grid cell location with respect to the locations of the measurement sites used in the "kriging" analysis). This approach does not address the problems associated with differences in "over-water" vs. "land-based" precipitation and meteorology.

Level Two estimates will attempt to decrease the uncertainty in the wet deposition estimates by using measured high-resolution precipitation data, derived from NWS Weather Surveillance Radar (WSR) observations. The interpolation of land-based precipitation depth over Lake Michigan ignores the surface forcings such as heat transfer, evaporation, frictional drag, and terrain induced flow modification the lake can impart on the overlying atmosphere. These surface forcings can change the overlying atmospheric stability and strongly affect precipitation processes. Changnon and Jones (1972) found average annual precipitation is 6% less over Lake Michigan than the surrounding land area. As in the Level One estimation technique, volume-weighted mercury concentrations will interpolated onto the 5 km over-water grid using the "kriging" technique. However, the gridded precipitation field will not be derived from a "kriging" of land-based precipitation gauge data. Rather, rainfall estimates for each grid cell will be determined using high-resolution rainfall estimates derived from WSR data by NASA's Marshall Space Flight Center (MSFC). The final wet deposition estimates would result from taking the product of the "kriged" concentration field and the WSR derived precipitation fields.

Level Three estimates of the wet deposition loading to Lake Michigan will offer the best degree of precision by utilizing "adjusted MSFC radar data". Although radar reflectivity is a direct measurement technique, it also has some inherent uncertainties. The empirical relationship between reflectivity factor (Z) and rainfall rate (R) is based upon droplet size distributions, which may be event specific. Additional errors can result when vertical air motions exceed the raindrop terminal velocity, particularly in convective storms (Burgess and Ray, 1986). Several methods of "rain gauge calibration" of the MSFC radar data are currently being evaluated. Adjusting the MSFC radar data to reflect the land-based rain gauge measurements will allow for a more accurate representation of the localized deposition patterns observed over the lake surface due to a more accurate description of the distribution of precipitation across the domain during the time period of interest.

An assessment of the climatological representativeness of the LMMBP data set will also be completed. A preliminary investigation revealed that, in general, precipitation in 1994 around Lake Michigan was significantly less than the 30-year climatological average.

In fact, the Chicago area experienced the driest year in more than 30 years, receiving only 29.6 inches of precipitation in 1994. Monthly climatologically averaged mercury wet deposition estimates will be estimated using "kriged" monthly climatological-average precipitation depths rather than the measurements made during the LMMBP study.

This will provide a meteorological representative mercury contribution to Lake Michigan from wet deposition and will characterize the average impact of the urban areas in the southern portion of the lake. This data will form the basis on which future wet deposition measurements could be compared.

Task 2. Determine that portion of the atmospheric deposition loading of total mercury to Lake Michigan due to "dry deposition". This task includes: 1) the determination of dry deposition velocities and volatilization rates, and 2) the determination of vapor-phase concentrations in the air-water interface.

Level One - Vapor exchange across the air-water interface and particle dry deposition constitute the remaining portion of atmospheric deposition not addressed in Task 1. Studies have shown that a significant mass of atmospheric contaminants, monitoring site data using an interpolation scheme called kriging. First, the ambient concentration values will be interpolated across Lake Michigan using the aforementioned kriging" technique, to obtain an estimate of "average concentration" for each grid cell at 5 km resolution. The deposition velocity for each point over the lake will be calculated using meteorological data provided by NOAA-GLERL. The final dry deposition estimate of each grid cell would result from taking the product of the "kriged" concentration field and calculated deposition velocity. Uncertainties in this method will be based on uncertainties in the measurement and analysis of the samples, plus the uncertainties due to the interpolation technique.

Level Two - In recent years the UMAQL has done considerable work in the development of a deposition model (Pirrone *et al*., 1995a,b) which takes into consideration the important mechanisms involved in the transfer of atmospheric contaminants to a receptor water surface. Recent work was successful in calculating the atmospheric input of contaminants to Lake Michigan during the Lake Michigan Urban Air Toxics Study (LMUATS) in the 1991 (Pirrone *et al*., 1995a,b), the Atmospheric Exchange Over Lakes and Ocean Surfaces Study (AEOLOS) in 1994 (Vette *et al*., 1996), and to Lakes Huron, Erie and St. Clair during two pilot studies carried out in the 1992 and 1994 (Pirrone *et al*., 1995c; Keeler and Pirrone, 1996). The results obtained during these studies have shown that due to large spatial and temporal variability of parameters (i.e., particle deposition velocity, Henry's law constant, gas-particle partitioning coefficient, ambient concentration, meteorological parameters) governing the transfer mechanisms of atmospheric contaminants, the deposition flux and gas exchange rate may vary by several orders of magnitude during the over-water transport.

Parameterizations from this model will be used by the UMAQL modelers in conjunction with the NOAA-GLERL 5 km over-water meteorological data to improve our understanding of the effects of different meteorological conditions on dry depositon processes to Lake Michigan.

Michigan

Analysis Level	Method to Obtain Gridded Concentration Field	Method to Obtain Gridded Precipitation Fields	Time Resolution of Deposition Estimates
Level One	Kriging of site data	Kriging of NWS data	Monthly/annual
Level Two	Kriging of site data	WSR radar	Monthly/annual
Level Three	Kriging of site data	Adjusted WSR radar	Monthly/annual

The UMAQL team will work closely with the LMMBP modelers to determine how best to incorporate this deposition module into the mass balance model for use in future load reduction studies. Extensive experience in deterministic and numerically modeling coupled with extensive experience in gridding both meteorological and emissions data will allow the UMAQL Team to efficiently communicate with the whole lake water modelers. Coupling the atmospheric models together with the lake hydrodynamic models will be a much more efficient process if both atmospheric and water modelers can communicate in an effective manner.

As was the case for the wet deposition estimates discussed under Task 1, a quantitative estimate of the uncertainties in these estimates will be included with the final results.

5. Personnel Descriptions

Gerald J. Keeler Ph.D. - Dr. Keeler presently holds an appointment as an Associate Professor in the Department of Environmental and Industrial Health as well as in the College of Engineering in the Department of Atmospheric, Oceanic, and Space Sciences, at the University of Michigan in Ann Arbor. He is also the Director of the UMAQL which he established in 1990. Dr. Keeler has extensive experience in planning, conducting, and managing large field studies aimed at understanding air quality and environmental problems. His focus has been on the measurement and modeling of atmospheric contaminants focusing on trace elements including mercury. He has been involved in research and monitoring programs in many parts of the United States and Canada. In 1991 he was the Principal Investigator for the Lake Michigan Urban Air Toxics Study (LMUATS) jointly performed by the UMAQL and USEPA-NERL. The LMUATS was the first study to investigate the importance of the Chicago/Gary urban/industrial area on toxic deposition to Lake Michigan (Keeler, 1994). Since 1991, Dr. Keeler has been a leader in atmospheric mercury research and methods development. His extensive experience in atmospheric mercury led to Dr. Keeler being invited to be on the Mercury Atmospheric Processes Expert Panel which included the top mercury scientists in the world. The UMAQL has been performing direct measurements of hazardous pollutant levels and deposition on Lake Michigan each year since 1991. The UMAQL has been investigating the transport and deposition of hazardous air pollutants across Michigan looking at a variety of semi-volatile organic carbons as well as trace elements. He will serve as coordinator for this interagency project and be responsible for the mercury modeling and interpretation.

Thomas M. Holsen, Ph.D. - Dr. Holsen is currently an Associate Professor and the Associate Chairman of Environmental Engineering Division in the Chemical and Environmental Engineering Department at Illinois Institute of Technology. His research interests include the environmental chemistry, transport, transformations and fate of hydrophobic organic chemicals in the Great Lakes. Recent research has focused on the development of instruments and techniques to measure the dry deposition of toxic compounds to natural surfaces. He is currently a co-principal investigator on three USEPA funded projects investigating the deposition of toxic chemicals in the Great Lakes region. He has published extensively on the absolute and relative importance of atmospheric deposition of toxic substances to and their cycling within the Great Lakes. He was a critical reviewer of the Identification of Sources section of the Great Waters Report to Congress for 1993. He has over 40 publications and has successfully supervised research projects sponsored by the USEPA, OSWR, and HWRIC.

Frank J. Marsik, Ph. D. - Dr. Marsik currently holds an appointment as a Post-doctoral Research Fellow in the Department of Environmental and Industrial Health at the University of Michigan in Ann Arbor. His doctoral research focused on the micrometeorological aspects of earth-atmosphere turbulent exchange processes. He has extensive

experience in planning and conducting micrometeorological support for various air quality field programs. Among the projects in which Dr. Marsik has participated are the 1990 Lake Michigan Ozone Pilot Study, the 1991 LMUATS, as well as the 1992 and 1993 forest-atmosphere exchange measurement campaigns associated with the USEPA's Southern Oxidants Study. He has most recently been working with scientists at NOAA's Atmospheric Turbulence and Diffusion Division on methods development related to surface mercury flux/deposition measurements.

Matthew S. Landis, M.S. - Mr. Landis is a Ph.D. student at the University of Michigan and currently serves as a graduate research assistant at the UMAQL. His MS research focused on development and evaluation of inorganic wet deposition collection and analysis methods. He has extensive experience in conducting and evaluating field air sampling projects. While with the Pennsylvania Department of Environmental Resources Bureau of Air Quality, Mr. Landis worked in conjunction with an USEPA-NEIC investigation on inorganic emissions from a hazardous waste recycling facility and with a mobile analytical laboratory study of organic emissions from point sources. He has participated in the 1994-95 AEOLOS intensive studies on Lake Michigan, the 1995 South Florida Atmospheric Mercury Project, and has coordinated the atmospheric mercury component of the LMMBP study. In addition, Mr. Landis conducted the trajectory analysis portion of the 1992-93 Trace Element Transport and Deposition Study sponsored by the Adirondack Lake Sampling Survey in collaboration with Dr. Ilhan Olmez at the MIT Nuclear Reactor Laboratory. His Ph.D. research is focusing on the long-range transport, in cloud processing, and wet deposition of inorganic trace elements to the Great Lakes.

B. Model Description

1. Researcher Responsibilities - Dr. Gerald J. Keeler, Principal Investigator for this project, will be responsible for oversight of the modeling phase of this project. Dr. Keeler will also be responsible for all communications between the UMAQL and USEPA QA/QC Officers. Dr. Frank Marsik will be responsible for meteorological data verification and consistency analysis. Matthew S. Landis will be responsible for the preparation of input data, performance of deposition model runs and interpretation of results.

2. Model parameters - The wet deposition estimation model will be written in SAS and will utilize the variogram and krige2d procedures. A detailed description of the SAS 6.12 implementation of the variogram and kriged procedures and the main equations can be found in the SAS Institute Inc., SAS/STAT® Technical Report: *Spatial Prediction Using the SAS System*, SAS Institute, Inc., Cary, North Carolina, 1996. 80 pp.

   The dry deposition estimation model will consist of two separate linked models. The first model will be written in SAS and will utilize the variogram and krige2d procedures to estimate particulate phase and vapor phase mercury concentrations onto the NOAA-GLERL 5 km over-water grid. The second model will be written in FORTRAN 77 and will use the mercury concentration estimates generated in the first model and high resolution over-water meteorological data supplied by NOAA-GLERL to estimate particle dry deposition.

3. Computer Aspects - A typical wet deposition model run for one-year over Lake Michigan at 5 km/1 month resolution takes approximately 30 CPU minutes on an IBM compatible PC (with a 200 megahertz 32 bit processor and 64 megabytes of RAM).

   A typical dry deposition model run for one year over Lake Michigan at 5 km/1 hour resolution takes approximately 6 CPU hours on a Sun Sparc 20 Workstation (with a 100 megahertz 64 bit processor and 48 megabytes of RAM).

4. Data Quality - The input data used for the modeling studies associated with this project will

be obtained from three major sources: (i) National Climatic Data Center (NCDC) in Asheville, North Carolina; (ii) NOAA-GLERL in Ann Arbor, Michigan; and (iii) the UMAQL in Ann Arbor, Michigan. The NCDC provided the TD3220 digital database, which includes NWS cooperative station precipitation depth. The NOAA-GLERL provided high resolution over-water Lake Michigan meteorological data. The UMAQL provided particulate phase mercury, vapor phase mercury and mercury in precipitation data collected during the USEPA, GLNPO sponsored Lake Michigan Loading Study. Preliminary QA/QC was performed on these data sets by the respective sources. The UMAQL visually interrogates all of the input chemical and meteorological data sets for consistency and accuracy prior to use.

C. Model Development

1. Code Development and Maintenance - The SAS® System is an integrated system of software providing complete control over data access, management, analysis, and presentation. SAS Version 6.12 was developed and tested by the SAS Institute, Inc. The Institute is a private company devoted to the support and further development of its software and related services.

   The dry deposition models for this project are presently being developed by the UMAQL. During the code development process, the UMAQL will keep complete records of model development, modifications made to the code, and code validation procedures. Model development records will include: (i) model assumptions; (ii) model parameter values and sources; (iii) changes and verification of changes made in the code; (iv) actual input used; (v) output of model runs and interpretation; and (vi) validation of the models.

2. Model Documentation - Full documentation for SAS 6.12 is available from the SAS Institute, Inc., *SAS Companion for the Microsoft Windows Environment, Version 6, First Edition.* Documentation for the Variogram and Krige2d procedures and the main equations can be found in the SAS Institute, Inc., SAS/STAT® Technical Report: *Spatial Prediction Using the SAS System,* SAS Institute, Inc., Cary, North Carolina, 1996. 80 pp.

   The UMAQL will provide complete documentation for the dry deposition model being developed as part of this project. The documentation will include: (i) the equations on which the model is based; (ii) the underlying assumptions; (iii) the boundary conditions that can be incorporated into the model; (iv) the method used to solve the equations; and (v) the limiting conditions. The UMAQL will also include instructions for operating the code including instructions for preparing data files, programmer's instructions, and computer operator instructions.

3. Code Verification - The SAS Institute, Inc. performed all code verification associated with SAS Version 6.12. Verification for the dry deposition model will be preformed by the UMAQL. The objective of the code verification process is to verify the precision and accuracy of the computational algorithms used to solve the governing equations and to assure that the computer code is fully operational.

4. Code Documentation - The SAS Institute Inc. performed documentation of the SAS Version 6.12 code. Documentation of the dry deposition model code will be preformed by the UMAQL. Code documentation will include model specifications; model descriptions, description of routines; and description of databases. The UMAQL will carefully inspect all model code developed as part of this project to reveal potential programming or logical errors. Comprehensive internal code documentation will also be incorporated into each of the models to aid in code development and maintenance, model documentation, and code verification.

D. Model Validation

Model validation is the comparison of model results with numerical data independently derived from environmental observations. Since the models

currently under development will estimate over-water atmospheric deposition to Lake Michigan, where few observations were made, it will be very difficult to validate these models. The UMAQL will make every effort to use what data is available to evaluate the mercury deposition models. Comparisons with other literature estimates will be performed when possible.

E. Record Usage and Management

1. Data records - All data generated by the UMAQL will be recorded in electronic format. All databases are backed up either to floppy disks, 8-mm tape, or removable hard-drive media, which are stored in different locations.

2. Records Management System - A master directory, LMMBP, will be created to hold all data. Separate subdirectories will be created for FINAL results. A complete description of the data directory structure will be included in a 'readme' file located in the master directory.

3. Records Validation - Electronic records produced during the course of the project will be stored in separate directories reserved for each individual participant. Computer files are manually validated by visually checking approximately 10% of the data records for accuracy. Record dates will be automatically available on all computer databases.

4. Record Identification, Indexing, and Retention - All database files will be identified by filename and subdirectory structure. Final data records will be retained on the computer drive until reports and publications are written and accepted, or throughout the length of the project, which ever is longer. After completion of the project, all electronic data will be duplicated on tape or removable hard-drive media and stored in replicate for the life of the tapes. Printed data shall be stored for a period five years after conclusion of the project.

5. Records Distribution and Storage - Only final data records will be distributed outside the UMAQL. These records will be prepared by the data manager and Matthew S. Landis, and will be carefully reviewed by Dr. Gerald J. Keeler before distribution and reporting. Interim storage of preliminary data records is described above.

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Atmospheric Loadings of PCBs, TNC, and Atrazine

Principal Investigator: Keri C. Hornbuckle, SUNY-Buffalo
Co-Principal Investigator: Joseph V. DePinto, SUNY-Buffalo
Project Officer: Angela Bandemehr, USEPA, GLNPO

A. Project Planning and Organization

1. Introduction - This project to calculate atmospheric deposition estimates for PCB congeners, TNC, atrazine, nitrogen and phosphorus to Lake Michigan is in support of the larger LMMBP. The LMMBP is a multi-investigator, multi-agency project designed to provide future guidance for toxic load reduction efforts in Lake Michigan. Through oversight by the GLNPO, the project includes monitoring field work, chemical process research, data integration, and modeling of the transport, fate and bioaccumulation of a suite of potentially harmful compounds in Lake Michigan. The four main goals of the LMMBP include:

    1. To identify relative loading rates of critical pollutants from tributaries, atmospheric deposition, and contaminated sediments in order to better target future load reduction efforts and to establish a baseline loading estimate to gauge future progress.

    2. To develop the predictive ability to determine the environmental benefits of specific load reduction scenarios for toxic substances and the time required to realize those benefits.

    3. To evaluate the benefits of load reductions from existing environmental statues and regulations.

    4. To improve our understanding of key environmental processes which govern the cycling and bio-availability of contaminants within relatively closed ecosystems.

    The Atmospheric Modeling team, consisting of researchers at the SUNY at Buffalo, Rutgers University, and the Chesapeake Biological Laboratory, will accomplish these objectives by providing atmospheric loading estimates for PCBs, TNC, atrazine, nitrogen and phosphorus. The SUNY team will utilize chemical and meteorological data provided by the LMMBP monitoring efforts, chemical data collected by the SUNY team aboard the Lake Guardian in July, 1997, and meteorological modeling results from the NOAA-GLERL. This document will detail the SUNY team's three-tiered approach to the loading estimates and quality control efforts used in collecting, managing, and interpreting data.

2 Project Hypothesis - We hypothesize that the magnitude of atmospheric deposition of semi-volatile organic compounds, nitrogen and phosphorous to Lake Michigan is dependent on proximity to major industrial centers (spatial factors) and seasonal meteorological/ hydrometeorological trends (temporal factors).

3. Project Objectives

    A. To summarize the current knowledge of atmospheric depositional processes and loadings of the target chemicals to Lake Michigan. Atmospheric deposition processes and loading includes wet deposition; dry particle deposition and; gas exchange (absorption and volatilization).

    B. To summarize and present data quality based on reported laboratory and field quality control sample results; suitability for loading estimates and; comparability with other available data.

    C. To estimate atmospheric deposition and loadings of the target compounds to Lake Michigan with respect to: spatial (e.g.

north-south) variability and; temporal (seasonal, monthly) variability.

D. To calculate the uncertainty associated with the atmospheric deposition and loading estimates for the target compounds.

E. To provide the loading estimates in a format accessible and useful to the whole lake mass balance modeling effort.

4. Project Description - Semi-volatile organic compounds, nitrogen and phosphorous enter Lake Michigan via washout in precipitation, dry deposition of contaminated particles, and vapor exchange, as well as through tributary, industrial effluents and other direct sources. The relative importance of all these chemical inputs to the lake, especially atmospheric inputs, are poorly understood for nearly all chemicals. This poses a critical problem because atmospheric inputs exert a very strong influence in our ability to predict chemical behavior. For example, Endicott *et al.* (1992) described a whole lake mass balance model, called MICHTOX, for PCBs in Lake Michigan. Their intention was to predict the accumulation of PCBs in fish under a number of remediation scenarios. One of their conclusions was that under a no-action scenario, PCBs in trout are expected to decrease by half in about five years. This prediction of rapid decline is caused by the rapid removal of PCBs from the lake by volatilization - an output that the model estimated to exceed all other losses, even burial to the sediments. Unfortunately, the volatilization rates estimated have significant uncertainty associated with them. Hornbuckle *et al*. (1995), using a modeling approach supported by a large air and water sampling program, reported volatilization loss of 520 kg for the northern three-quarters of the lake. Pearson *et al*. (1996), extrapolated these results to the southern quarter of the lake and reported total volatilization losses of about 680 kg. Furthermore, recent unpublished work by Zhang (1996) has indicated that the southwestern region of the lake, near the heavy industries of Gary and Chicago, experiences very large gaseous and particulate deposition of PCBs. This deposition exceeds volatilization and the atmosphere no longer represents a sink but a source of PCBs to Lake Michigan. All this recent work indicates that the ability of models like MICHTOX to predict long-term chemical behavior depend on high quality estimates for atmospheric exchange.

Meeting the project objectives described above will require development of new interpolation methods not previously used in atmospheric deposition calculations. Interpolation of chemical concentrations (gases, particle-bound, and in rain), rainfall, particle deposition is the most difficult and time-consuming problem that this project addresses. Interpolation in time is difficult because of the sampling limitations facing the LMMBP monitoring efforts. The necessity of composite gas-phase samples makes temporal interpolation of gas-phase samples especially difficult. Interpolation in space is difficult because of the very large area of the lake and the small number of sampling stations (relative to the observed spatial concentration variability). This project uses a four-tiered approach to the space/time interpolation. Level One represents the lowest level of difficulty and is reflective of techniques currently used by researchers in the field. Levels Two, Three, and Four utilize new techniques that require progressively more computational rigor.

Level One includes calculations of the instantaneous deposition fluxes at each of the LMMBP sites. Preliminary values for Level One calculations were presented in the mid-term report of July, 1997. The methods summarized by Vlahos *et al* (1995) and by Hoff *et al* (1996) are applied.. An assessment of the quality and representativeness of individual samples and sampling sites has also been undertaken. This work is necessary for all flux calculations and will continue until all the USEPA-approved data has been received and reviewed.

Level Two includes an interpolation of the concentration data to describe over-lake values on a monthly time scale. Concentrations in rain over the lake are interpolated using kriging or inverse distance weighting. Concentrations are

determined for each cell in the 5 km grid domain. Chemical concentrations in rain are interpolated in time on a monthly basis as required by the monthly samples available for most of the target chemicals. Wet deposition is determined by multiplying these concentrations by the rainfall volume falling in each cell, at monthly intervals. Rainfall over the lake has been estimated using NWS rain gauge data, radar data and kriging techniques by Dr. Jerry Keeler's group (See QAPP, Keeler and Landis, August, 1997). For consistency, we will be using the same rainfall data set. Dry particle deposition is estimated in a similar fashion: chemical concentrations on particles are interpolated in space using inverse distance weighting or kriging; particle deposition is estimated using a method developed by Keeler and Landis.

Gas-deposition is the largest but least uncertain atmospheric loading for PCBs and TNC. It is the largest deposition flux for atrazine in all seasons except springtime. For the Level Two calculations, gas deposition will be estimated by interpolating chemical fluxes and chemical concentrations from the land sites across the lake using Geographic Information Systems (GIS) and a inverse distance or kriging method to interpolate in space. Level Two calculations will only be estimated on a monthly basis, reflective of the sample composite periods.

Level Three estimates whole lake loadings on an hourly basis for the gas-phase compounds. This level involves an interpretation of sources (non-point) of chemicals to the air over Lake Michigan. Such a fine time scale is not possible for wet and dry deposition of the PCBs, TNC, and atrazine because of the large uncertainties in the data and the manner of sample collection (monthly rain collection rather than event based). Interpolation of gas-phase concentrations is possible because of their dependence on highly resolved meteorological conditions.

Gas-phase concentrations are temporally interpolated on an hourly basis as a function of 1) water temperature, 2) land surface temperature, 3) wind direction, and 4) wind speed. Water and land surface temperatures affect the equilibrium distribution of chemicals between air and surfaces. The equilibrium distribution is expected to affect but not necessarily control gas-phase concentrations. Wind direction determines whether the water surface or the land surface temperatures should be used in the prediction. Wind direction may also be used to predict the importance of local sources (or land vs. water sources). Wind speed may be an important predictor due to mixing with background air or resuspension of contaminated dust. Meteorological data for this interpolation includes the results of the NOAA-GLERL hydrodynamic model (Schwab and Beletsky, 1998) and data collected at the eight sampling sites on land around the lake. A complete description of the temporal interpolation of gas-phase chemical concentrations is included in the appendix.

Spatial interpolation across the lake (at hourly time scale) will proceed as in Level Two. Samples collected on the Lake Guardian during the LMMBP field season will be included as a verification of the interpolation and/or as additional sites for spatial interpolation. Because a preliminary review of the Lake Guardian samples indicted greater than expected imprecision between the samples collected at a location/time using different sampling apparatuses, a field study of these different sampling apparatuses was conducted in Lake Ontario in July, 1997 (see Sections 3 and 4). The Lake Ontario samples will be used to assist in the interpretation of the Lake Michigan Lake Guardian data. The Lake Ontario samples will not be used in the interpolation work directly.

Level Four is the incorporation of the flux calculations into a coupled deposition and emission modeling framework. The atmospheric modeling group will be designing a system for coupling the gas-exchange model with the lake toxics model. The Level Four work will include a set of screening models to examine the dynamic interactions between air and water with respect to toxic chemical deposition. These screening models are necessary because the

spatial interpolation of gas-phase concentrations, as described in Levels One, Two, and Three, ignore interaction of the air with the water below it. This is not realistic and may provide inaccurate estimates of gas-phase concentrations.

5. Personnel Descriptions

Keri C. Hornbuckle, Ph.D. - Dr. Hornbuckle is an assistant professor of environmental engineering in the Department of Civil, Structural and Environmental Engineering at the University at Buffalo. Dr. Hornbuckle's research interests concern the fate and transport of organic pollutants in natural systems, with special focus on atmospheric processes that control long-term ecosystem exposure to potentially toxic and persistent contaminants. Dr. Hornbuckle's research activities include field work, analytical chemistry, and fate and transport modeling. Dr. Hornbuckle will oversee the transfer of information and organize all communications required by this project, including exchange between investigators, consultants, the mercury project team, the project director at GLNPO, and the whole-lake mass balance modeling team. She is responsible for the chemical modeling and interpretation.

Joseph V. DePinto, Ph.D. - Dr. DePinto is Professor of Civil Engineering and Director of the Great Lakes Program at the SUNY at Buffalo. In the broad area of understanding and quantifying the impacts of pollutants on natural aquatic systems, Dr. DePinto has received over $4 million in grants and contracts. These studies have led to over 80 scientific publications in this area and the direction of 34 Master's theses and 10 Ph.D. dissertations. Dr. DePinto has been a part of the Great Lakes research community for twenty years. During that time he has conducted research throughout the Great Lakes basin on such topics as nutrient-eutrophication, toxic chemical exposure and bioaccumulation analysis, contaminated sediment analysis and remediation, biotic trophic structure and functioning, and watershed, tributary, whole lake modeling. He has also had considerable experience in exposure analysis of contaminants through deterministic modeling. For example, he was a member of the modeling team that undertook the development and application of the integrated exposure model for PCBs in Green Bay, Lake Michigan.

Two principal consultants, Eisenreich and Baker, are named on this proposal as an indication of their commitment and involvement to the project. Their role in the project is provide guidance to the general project and to carry out specific duties as described below.

Steven J. Eisenreich, Ph.D. - Dr. Eisenreich is Professor of Environmental Chemistry and Chairman of the Department of Environmental Sciences at Rutgers University. His research interests include the environmental chemistry, transport, transformations, and fate of hydrophobic organic chemicals in the Great Lakes. He has published extensively (~110 publications) on the absolute and relative importance of atmospheric deposition of toxic substances to and their cycling within the Great Lakes. He was instrumental in establishing the Integrated Atmospheric Deposition Network (IADN) in the Great Lakes region, assisted in development of the concepts for the Great Waters Program of the CAAA-90, is co-author of the Relative Loadings section of the Great Waters Report to Congress for 1993, and has contributed to the scientific background report for the 1995 Report to Congress.

Joel E. Baker, Ph.D. - Dr. Baker is an Associate Professor at the University of Maryland's Chesapeake Biological Laboratory in Solomons, Maryland. Dr. Baker's research interests center about the transport of hydrophobic organic contaminants in the atmosphere and in surface waters. His studies in the Great Lakes have documented the importance of volatilization and sediment resuspension in the lake-wide mass balances of organic contaminants. He is one of the original collaborators of the Chesapeake Bay Atmospheric Deposition Study and recently co-authored the report Relative Loadings of Toxic Contaminants and Nitrogen to the Great Waters for the USEPA's Great Waters Program.

Mark L. Green, M.S. - Mr. Green is a Ph.D. student at the University at Buffalo. He has extensive experience in the use of stochastic and probability methods in high performance computing. He is fluent in several programming languages, including Fortran and C and is proficient in the use of Arc/Info and GIS. He has worked on a wide variety of computer modeling-related projects in the geotechnical and environmental fields. He received a B.S. in chemical engineering from the University at Buffalo. His masters thesis, from the University of Buffalo, Department of Civil Engineering, is titled, "Transport of Trichloroethylene Vapors in a Random Porous Medium." His Ph.D., "Cross-media Coupling of Mass Balance Models" focuses on the interfacing of large and independent computer models that operate under different spatial and temporal scales.

Sondra M. Miller - Ms. Miller is a masters student at the University at Buffalo Department of Civil, Structural and Environmental Engineering. She has a B.S. in civil engineering from University of Buffalo and has participated in research-related activities for over three years. As an undergraduate, Ms. Miller was selected as an National Science Foundation fellow and conducted research on biofilms at the University at Buffalo Industry/University Cooperative Research Center for Biosurfaces.

6. Researcher Responsibilities - Dr. Keri Hornbuckle, Principal Investigator for this project, is responsible for oversight of the modeling and data collection aspects of the project. Dr. Hornbuckle is also responsible for all communications between the participants, the USEPA project director and QC/QA officers, the mercury project participants, and the project consultants. Dr. Joseph DePinto is responsible for communications with the whole-lake modelers and oversees the GIS modeling applications. Dr. Steve Eisenreich is responsible for the use of AEOLOS data in this study and will assist in the interpretation of nutrient concentrations in rain. The results of the AEOLOS study will be used primarily for additional verification of the spatial interpolation model. The AEOLOS data will not be processed through the same quality control procedure as the LMMBP database, so cannot be used directly in the interpolation models. Dr. Baker will assist in the interpretation of chemical concentrations in rain. Mr. Mark Green is responsible for the preparation of input data, development of the concentration interpolation models, and interpretation of modeling results. Ms. Sondra Miller is responsible for instantaneous flux calculations, field sampling and analysis, and interpretation of the Lake Guardian data.

B. Model Description

1. Model Parameters - Database manipulation, temporal interpolation and regressions will be written in FORTRAN and C computer languages. Preliminary regression and interpolations of gas-phase concentrations are performed in Excel MSOffice 97. Results for wet and dry particle deposition and gas concentrations are spatially interpolated and displayed in Arc/Info 7.01 (Kreis, 1995).

   Rainfall and particle deposition will be modeled in SAS as described in Keeler and Landis (1997).

2. Computer Aspects - The site database assembly for eight sites is expected to require 180 CPO minutes on Sparc 10 Workstation (64 RAM, 55 Megahertz Processor). The site temporal interpolation for eight sites requires 10 CPU minutes and the site spatial interpolation requires 5 CPU minutes on Sparc 10 Workstation.

3. Data Quality - The data used in this study is obtained from eight major sources: 1) The LMMBP QA Officer Louis Blume. For data that has not yet passed QC, data from the generating laboratories will be used. This preliminary data is from the Illinois State Water Survey (ISWS), Rutgers University, The Chesapeake Biological Laboratory, and the Indiana University. 2) Meteorological data is from NOAA-GLERL, the UMAQL and the LMMBP. For meteorological data from the LMMBP (site data) that has not yet passed QC, preliminary data is gathered from ISWS and Indiana University. 3) Some Lake

Guardian data is from the University at Buffalo Environmental Engineering Laboratories.

Quality control on this data was generally provided by the originators. An overview assessment of the quality of raw data has been undertaken. QC efforts for the University at Buffalo data is reported below. Final loading estimates provided to the modelers will be based on USEPA verified data.

4. Model Development - The modeling approach for the temporal interpolation of gas-phase concentrations is the most computer and person-time intensive aspect of this work. In brief, the approach involves: 1) an interpolation of the discrete and composite chemical data over time. This interpolation involves fitting the data to a regression model using surface water temperature, air temperature, wind direction and wind speed as input parameters. The monthly data will then be described on a much finer temporal resolution. To complete this regression, it is necessary to separate the air arriving at each sampling station with respect to its over-water or over-land origins. Using wind direction to fractionate the sampled air, the temperature regime used for the regression is either the surface water temperature or the air temperature measured at the site. A more detailed description of this approach is found in the appendix.

5. Model Validation - Model validation is the comparison of model results with numerical data independently derived from environmental observations. Over 65 air samples were collected by the LMMBP aboard the Lake Guardian during the 1994-95 season. Approximately 20 more samples were collected in the southern portion of the lake in 1993-94 by AEOLOS. The data from these samples will be used to test the validity of the model. This approach is most useful for gas-phase PCB and TNC. This is fortunate because the interpolation procedure to be applied is the most finely resolved and most rigorous for these compounds. Concentrations of atrazine were near or below detection limits. No measurements of nitrogen or phosphorus were measured on the vessel and few rain events were captured.

6. Record Use And Management - All data generated by this project is stored electronically in three separate hard drives and backed up on a tape that is stored separately. Data that is generated elsewhere but used on this project is stored as above and also on floppy disks. A master directory, containing only original files is stored on a hard drive.

   Computer calculations are manually and randomly calculated at regular intervals. Record dates are automatically available on all computer databases.

   After completion of the project, all electronic data will be duplicated to a compact disk as a permanent archive. Printed data will be stored for at least five years after the completion of the project.

7. Model Output/Products - Loading and/or concentration data will be provided to the whole lake mass balance modelers in a manner that is convenient for them. At this time, we intend to provide concentration estimates for gas-phase PCBs and TNC on a daily basis over a 5 km grid. Gas-phase atrazine will be provided on a monthly basis for the whole lake (average). Loadings of wet and dry particle deposition will be provided on a monthly basis for all chemicals. These estimates, and appropriate determination of uncertainty, will be provided in ASCII or cdf file format electronically (ftp) as completed or at the end of our funding period, which ever is earlier.

C. Replicate Air Sampling on the Lake Guardian

1. Project Description - A survey on the Lake Guardian is necessary to aid the atmospheric modelers responsible for interpreting the atmospheric data gathered by the LMMBP. During the LMMBP field season, over 65 air samples were collected aboard the Lake Guardian. Duplicate samples were collected at about a 5% rate. These duplicates exhibited an unusually large relative mean difference for the

organics concentrations. The large mean differences seriously reduce the LMMBP's confidence in the samples, and therefore, reduce the utility of those expensive and valuable samples. The purpose of this summer's survey is to repeat the duplicate sampling in hopes of illuminating the problem that occurred originally.

Vapors and particles will be collected using high volume air samplers equipped with XAD and glass fiber filters mounted on the bow of the Lake Guardian. Three hivols will be operated simultaneously. One will be on the deck of the bow. Two will be mounted on the yardarm. Each sample will run for 12 hours. This duplicate experiment will be repeated at least three times over four days. The number of samples is limited to the number of XAD cartridges available (10 at this time). Gas-phase and particulate phase organics will be sampled and analyzed in the manner described in the QAPP-Atmospheric Monitoring for the LMMBP and the Lakes Michigan and Superior Loading Studies. The exceptions to the sampling protocol are as follows: air samples will be collected in triplicate; each air sampler will be calibrated at the beginning of each sample; sampling flow rates will not be adjusted but recorded for each sample collected; samplers will not be turned on and off with the change in wind direction but run continuously over 12 hours. Meteorological and location information, along with other relevant metadata, will be recorded continuously.

Further details of the methods applied on this project are available in the LMMBP Methods Compendium (USEPA, 1997).

2. Sequence of Survey Tasks/Events - Air sampler are loaded to the vessel and secured to the bow.

    1. The two air samplers on the yard arm are checked for parts and operation.

    2. Clean lab space is established: aluminum foil covering a five ft lab bench.

    3. Freezer space established (16 ft^2).

    4. Air samplers cleaned and rinsed with acetone and water.

    5. XAD and GFF loaded, air samplers calibrated (for each sample collected).

    6. Wind speed, air temperature, surface water temperature, precipitation will be monitored hourly or as available.

    XAD and GFF will be changed and sampler flow rate measured at ~ 8 a.m. and 8 p.m. daily. XAD samples are wrapped (XAD still in cartridge) in combusted aluminum foil several times and stored in individual plastic bags in the freezer. Samples are transported from the ship to the lab in a cooler.

    Steps 5-8 will be repeated daily.

    Upon return to Buffalo, XAD and filter samples will be stored in a previously unused freezer until analysis.

3. Measurement/Data Acquisition - The experimental design follows the Great Lakes Water Quality Survey Study on Lakes Michigan, Huron, Erie, Ontario, and Superior (Warren, 4.29.97 Draft Plan) with the following exceptions:

    Nine XAD-2 samples, five polyurethane foam samples, and 10 glass fiber filter samples will be collected on the Lake Guardian while in Lake Ontario.

    The XAD-2 samples (critical samples) will be collected in triplicate using two samplers on a yard-arm and one on the bow. PUF samples (non-critical) will be collected in duplicate or as single samples, depending on the Lake Guardian schedule. Surface film samples (non-critical) may be collected to screen for hydrocarbon films on the water surface. Wipes of the ship deck surface (non-critical) may be collected to screen for PCBs adsorbed to the deck.

    Although the data collected here will support the data collected as part of the LMMBP work in

1994-1995, this work will be conducted on Lake Ontario. The change in lakes in inconsequential as this study is designed to test the sampling protocol used in the LMMBP.

The air samples will be analyzed for PCB congeners, and TNC.

4. Sample Handling and Custody Requirements - Each sample will be labeled with date, start and stop times, media type, and operator. All air samples are stored in freezers on the ship and at the University at Buffalo. Samples are transported to and from the ship on ice in a cooler by Hornbuckle and graduate students.

D. Sample Extraction and Analysis

1. Analytical Methods - Extraction, cleanup, and concentration of air samples collected on XAD-2 is described in detail in Harlin *et al.*, 1995. In brief, XAD air samples collected on the Lake Guardian are transferred to glass, foil-lined jars and sealed in plastic bags in a -10°C freezer until analysis. Samples are extracted with 50:50 acetone:hexane overnight. The resulting solvent solution is reduced to about 1 mL using a rotary evaporator. Interfering compounds are removed and analytes separated into different fraction with silica gel (3% deactivated). The first fraction (hexane) contains all PCBs and the pesticides HCB and DDE. The second fraction (40% DCM, 60%hexane) contains all PAHs and pesticides α and γ HCH, dieldrin, DDD, DDT, γ-chlordane, α-chlordane, and TNC. Fraction three (methanol) contains atrazine and two metabolites (deisopropylatrazine and deethylatrazine). The samples are then concentrated to the desired volume with a slow stream of ultra-pure nitrogen. Final volumes depend on sample matrix, site, and date. Each sample is spiked with a known amount of internal standard. Subsamples are then transferred to autosampler microvials for capillary GC-EC or GC-MSD analysis.

   Exceptions to the method described by Harlin and Surratt (1995) include:

   Samples will only be analyzed for PCBs, although all fractions will be retained for future analysis.

   - Gas Chromatography-Electron Impact Mass Spectrometry will be used instead of Ion Trap Mass Spectrometry.

   - PCB congeners 2,4,6-trichlorobiphenyl (#30) and 2,2',3,4,4',5,6,6'-octachlorobiphenyl (#204) are added as internal standards

   - All samples are spiked prior to extraction with PCB congeners 3,5-dichlorobiphenyl (IUPAC #14); 2,3,5,6-tetrachlorobiphenyl (#65); 2,3,4,4',5,6-hexachlorobiphenyl (#166) as surrogates

2. Quality Control - The data collected for this project will be analyzed and reported in a manner that assesses precision, accuracy, representativeness, completeness, and comparability with other projects.

   Precision, defined as the relative uncertainty about a given measurement, is assessed by replicate analyses. Precision will be monitored by the analysis of 10% of the extracts of the air samples split into two equal fractions and each analyzed as separate samples. All XAD/GFF air samples are measured in triplicate, with two collected on the yard-arm sampler and one on the bow sampler. Air samples collected with PUF/GFF are sampled individually.

   Accuracy, defined as the absolute uncertainty about the true value, will be assessed by surrogate spike recoveries in every sample and by spike experiments with performance standards. The compounds serving as surrogates will differ for each compound class. Surrogates for air XAD and GFF samples are added to the media prior to extraction. All compounds will be reported on a compound-specific basis (e.g. PCB congeners).

   Field blanks will consist of 10% of the samples collected. Air field blanks are XAD plugs and

filters carried to the field and returned to the laboratory unopened. Sample results will not be corrected for blank values; analyte concentrations in samples and blanks will be reported.

Comparability expresses the confidence with which one data set can be compared to another, either between laboratories or within a laboratory for different batches of samples. All data in this study will have internal comparability due to the use of self-consistent field and analytical procedures, and can be monitored by surrogate spike recovery performance. The manner in which the samples were collected and analyzed is designed to be highly comparable to the LMMBP data set collected on Lake Michigan in 1994-1995. Comparability between these data and other investigators' data will be dependent on the similarity of the field and analytical methods used between the studies. This can be determined by comparing accuracy measures. Data will be reported in units consistent with other studies of toxics in air.

Completeness is defined as the percentage of acceptable data needed to validate the study. It is calculated as the number of samples with concentrations above detection passing QA criteria divided by the number of samples analyzed having concentrations above detection multiplied by 100. Completeness for this study is set at 90%; reanalysis of a extract sample that fails QA will be performed. Sample data not meeting QA criteria will be flagged.

Samples will be collected in a manner that reduces external contamination (all equipment is solvent rinsed and dried prior to use, precombusted aluminum foil is used to seal samples) and prevents their misidentification. Where possible, air, water, soil, and vegetation samples will be collected simultaneously in order to improve comparability between media types. Upon collection, samples will be labeled by type, date, time, and replicate. An example of an air sample label: indicating an air sample collected on quartz fiber filter on July 1, 1997 at 1:45pm. Once collected, samples are tightly wrapped in precombusted foil, sealed in a plastic bag, and frozen at -10°C or lower. After collection, all samples will be protected from ultra-violet light.

The high volume air sampler will be calibrated in the field, prior to each sample, using the portable calibration unit bought from the airsampler manufacturer (Graseby/GMW).

A final report will be issued to the USEPA Project Officer upon completion of all sample analyses and data interpretation at the end of the project period. The final report will contain the complete data set and QA/QC results.

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F. Appendix - Proposed PCB Interpolation and Data Interpretation

Problem Statement - We have a collection of N sample masses collected from N sample volumes over a given period of sample time. In other words:

Total sample mass (M_{total})

$$M_{total} = \sum_{i=1}^{N} M_i$$

Total sample volume (V_{total})

$$V_{total} = \sum_{i=1}^{N} V_i$$

Total sample concentration (C_{total})

$$C_{total} = \frac{M_{total}}{V_{total}} = \frac{\sum_{i=1}^{N} M_i}{\sum_{i=1}^{N} V_i}$$

Since there are discrete sample times (one-hour intervals) at which meteorological parameters are known, a determination of where individual sample masses originated from can be utilized. Thus for the N discrete samples:

$$N = N^L + N^W$$

where N^L denotes number of discrete samples from land-based source and N^W denotes the number of discrete samples from water-based sources. Thus, expanding the series representation for the total sample concentration

$$C_{total} = \frac{MW_{PCB}\left(\sum_{i=1}^{N^L}\frac{P_i^{o\,L}}{T_i^L} + \sum_{i=1}^{N^W}\frac{P_i^{o\,W}}{T_i^W}\right)}{RN}$$

$$C_{total} = \frac{\sum_{i=1}^{N^L} M_i + \sum_{i=1}^{N^W} M_i}{\sum_{i=1}^{N} V_i}$$

Now converting the sample into an expression obtained from the ideal gas law we have

$$M_i = \frac{P_i^o\, V_i\, MW_{PCB}}{RT_i}$$

substituting

$$C_{total} = \frac{\sum_{i=1}^{N^L}\frac{P_i^{o\,L}\, V_i\, MW_{PCB}}{RT_i^L} + \sum_{i=1}^{N^W}\frac{P_i^{o\,W}\, V_i\, MW_{PCB}}{RT_i^W}}{\sum_{i=1}^{N} V_i}$$

We can now further simplify the total concentration expression by assuming that all discrete sample volumes are equal then

$$V_{total} = \sum_{i=1}^{N} V_i \qquad V_i = \frac{V_{total}}{N}$$

then

$$C_{total} = \frac{\frac{V_{total}\, MW_{PCB}}{RN}\left(\sum_{i=1}^{N^L}\frac{P_i^{o\,L}}{T_i^L} + \sum_{i=1}^{N^W}\frac{P_i^{o\,W}}{T_i^W}\right)}{V_{total}}$$

Finally, rearranging into a form that we can use for least squares fit for the unknown quantities of interest substituting

$$P_i^{o\,L} = \exp\left(= \frac{B^L}{T_i^L} + A^L\right)$$

$$P_i^{o\,W} = \exp\left(-\frac{B^W}{T_i^W} + A^W\right)$$

$$C_{total} = \frac{MW_{PCB}\left(\sum_{i=1}^{N^L}\frac{\exp\left(\frac{B^L}{T_i^L} + A^L\right)}{T_i^L} + \sum_{i=1}^{N^W}\frac{\exp\left(-\frac{B^W}{T_i^W} + A^W\right)}{T_i^W}\right)}{RN}$$

also, wind speed can be incorporated to account for enhanced transport at high wind speed. We assume an exponential power law relationship that has been used in the literature frequently:

$$Ws_{EFF}^L = 1 + \lambda_L\,(Ws_i^L)^{\eta_L}$$

$$Ws_{EFF}^W = 1 + \lambda_W\,(Ws_i^W)^{\eta_W}$$

Note these functions are valid for any wind speed value (zero wind speed results in an effective wind speed enhancement of one). Now substituting we get:

$$C_{total} = \frac{MW_{PCB}}{RN} \sum_{i=1}^{N^L} \frac{\exp\left(-\frac{B^L}{T_i^L} + A^L \right)}{T_i^L} \left[1 + \lambda_L \left(Ws_i^L \right)^{\eta_L} \right] +$$

$$\frac{MW_{PCB}}{RN} \sum_{i=1}^{N^W} \frac{\exp\left(-\frac{B^W}{T_i^W} + A^W \right)}{T_i^W} \left[1 + \lambda_W \left(Ws_i^W \right)^{\eta_W} \right]$$

The above equation uses the available data completely with no approximation. In order to solve for the required parameters we must approximate this equation with two average values

$$T_{AVG}^L = \frac{\sum_{i=1}^{N^L} T_i^L}{N^L} \qquad Ws_{AVG}^L = \frac{\sum_{i=1}^{N^L} Ws_i^L}{N^L}$$

$$T_{AVG}^W = \frac{\sum_{i=1}^{N^W} T_i^W}{N^W} \qquad Ws_{AVG}^W = \frac{\sum_{i=1}^{N^W} Ws_i^W}{N^W}$$

$$C_{total} = \frac{MW_{PCB}}{RNT_{AVG}^L} \left[1 + \lambda_L \left(Ws_{AVG}^L \right)^{\eta_L} \right] \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right) +$$

$$\frac{MW_{PCB}}{RNT_{AVG}^W} \left[1 + \lambda_W \left(Ws_{AVG}^W \right)^{\eta_W} \right] \exp\left(-\frac{B^W}{T_{AVG}^W} + A^W \right)$$

Units and parameter definitions

$$C_{total}\left[\frac{ng}{m^3}\right] \quad MW_{PCB}\left[\frac{ng}{mol}\right] \quad R\left[\frac{m^3 \cdot atm}{mol \cdot K}\right] = 0.08205783e-3$$

$$T_{AVG}^L [K] \quad Ws_{AVG}^L \left[\frac{m}{s}\right] \quad \lambda_L \left[\frac{s}{m}\right]$$

$$T_{AVG}^W [K] \quad Ws_{AVG}^W \left[\frac{m}{s}\right] \quad \lambda_W \left[\frac{s}{m}\right]$$

Derivatives with respect to parameters

B^L

$$C_{total} = -\frac{MW_{PCB}}{RN \left(T_{AVG}^L\right)^2} \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right) -$$

$$\frac{MW_{PCB}}{RN(T_{AVG}^L)^2} \lambda_L \left(Ws_{AVG}^L\right)^{\eta_L} \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right)$$

B^W

$$C_{total} = -\frac{MW_{PCB}}{RN \left(T_{AVG}^W\right)^2} \exp\left(-\frac{B^W}{T_{AVG}^W} + A^W \right) -$$

$$\frac{MW_{PCB}}{RN(T_{AVG}^W)^2} \lambda_W \left(Ws_{AVG}^W\right)^{\eta_W} \exp\left(-\frac{B^W}{T_{AVG}^W} + A^W \right)$$

A^L

$$C_{total} = -\frac{MW_{PCB}}{RNT_{AVG}^L} \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right) +$$

$$\frac{MW_{PCB}}{RNT_{AVG}^L} \lambda_L \left(Ws_{AVG}^L\right)^{\eta_L} \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right)$$

A^W

$$C_{total} = -\frac{MW_{PCB}}{RNT_{AVG}^W} \exp\left(-\frac{B^W}{T_{AVG}^W} + A^W \right) +$$

$$\frac{MW_{PCB}}{RNT_{AVG}^W} \lambda_W \left(Ws_{AVG}^W\right)^{\eta_W} \exp\left(-\frac{B^W}{T_{AVG}^W} + A^W \right)$$

λ_L

$$C_{total} = \frac{MW_{PCB}}{RNT_{AVG}^L} \left(Ws_{AVG}^L\right)^{\eta_L} \exp\left(-\frac{B^L}{T_{AVG}^L} + A^L \right)$$

λ_W

$$C_{total} = \frac{MW_{PCB}}{RNT^W_{AVG}} \left(Ws^W_{AVG}\right)^{\eta_W} \exp\left(-\frac{B^W}{T^W_{AVG}} + A^W\right)$$

η_L

$$C_{total} \frac{MW_{PCB}}{RNT^L_{AVG}} \ln\left(Ws^L_{AVG}\right) \lambda_L \left(Ws^L_{AVG}\right)^{\eta_L} \exp\left(-\frac{B^L}{T^L_{AVG}} + A^L\right)$$

η_W

$$C_{total} = \frac{MW_{PCB}}{RNT^W_{AVG}} \ln\left(Ws^W_{AVG}\right) \lambda_W \left(Ws^W_{AVG}\right)^{\eta_W} \exp\left(-\frac{B^W}{T^W_{AVG}} + A^W\right)$$

A very simple two-resistance model for partial pressure based volatilization/adsorption flux calculation

$$Flux = F_{PCB} = K_W \left(C_{PCB_W} - \frac{P^o}{H}\right)$$

$$\frac{1}{K_W} = \frac{1}{k_W} + \frac{RT}{hK_a}$$

where F_{PCB}[mol/(m^{2}s)] denotes the flux from water to air, k_A, k_W, and K_W [m/s] denote the water, air, and overall water mass transfer coefficient, H [Pam^3/(mol)] is Henry's law constant, R [8.314 Pam^3/(mol°K)] denotes the ideal gas law constant, C^W_{PCB} [mol/m^3] denotes the dissolved chemical concentration, and P° [Pa] denotes the chemical gaseous partial pressure in the atmosphere. In fugacity form

$$Flux = F_{PCB} = D_{AW}\left(f_W - f_A\right)$$

$$Z_W = \frac{I}{H} \quad Z_A = \frac{1}{RT}$$

$$D_A = k_A Z_A \quad D_W = k_W Z_W$$

$$\frac{1}{D_{AW}} = \frac{1}{D_W} + \frac{1}{D_A} \quad D_{AW} = K_W Z_W$$

These equations are identical to the partial pressure-based model. As shown by Mackay *et al*., a total air-water exchange mass balance can be assembled to give the net water to air flux as:

$$N = D_{AW}\left(f_W - f_A\right) - f_A D_R - f_A D_P - f_A D_D$$

if the net flux (N) is zero and steady-state is achieved

$$\frac{f_W}{f_A} = 1 + \frac{(D_R + D_P + D_D)}{D_{AW}}$$

where D_R denotes the wet deposition dissolution transport parameter, D_P denotes the dry deposition transport parameter, D_D denotes the wet deposition particle scavenging transport parameter, and D_{AW} denotes the overall water transport parameter [mol/(m^{3}sPa)]. This equation shows that air and water will tend to approach a steady-state but a non-equilibrium condition occurs.

Similar equations can be derived for the land-based source, which will give us the means to estimate land and water surface flux values for the system. Once the fugacity, (partial pressure), distribution is estimated, a linear regression can be also used to estimate the enthalpy change for each domain.

Important assumptions and approximations:

1. No consideration of analytic or sampling error is accounted for.

2 Ideal gas law is valid were implemented (very dilute samples).

3 The molecular weight used is an approximation (average of many congeners).

4. The air temperature at the site (local meteorological data) is used to approximate the local land surface temperature.

5. The closest cell surface water temperature (Schwab data) approximates the water surface temperature.

6. The hourly sample volumes are assumed constant and steady for all sites.

7. The land- and water-based sample partial pressures are approximated by using land- and water-based average temperatures.

All quantities are known in the final equation except the land- and water-based partial pressures. At first glance, it seems that all site data can be combined to estimate the land- and water-based partial pressure as there should not be significant local effects (essentially same site characteristics), obviously this is not true for the Chicago area. I think it would also be very interesting to investigate each individual site to see if this preliminary assumption holds true. This analysis incorporates not only wind direction, but also land- and water-based temperature variability. If the ambient air sampled at the sites exhibits local equilibrium tendency and the sorption-desorption reactions are fast enough, then the temperature gradient should dominate the fate and transport of PCBs.

From the Clausius-Clapeyron equation we have:

$$\frac{dP^o}{dT} = \frac{\Delta H_{12}}{T\Delta V_{12}}$$

approximating the volume change and applying the ideal gas law

$$\Delta H_{12} = V_{gas} - V_{liquid} \approx V_{gas}$$

$$V_{gas} = \frac{RT}{P^o}$$

Thus, substitution and transformation of variable, we obtain:

$$\frac{d(\ln P^o)}{dt} = \frac{\Delta H_{12}}{RT^2}$$

separating variables and integrating yields:

$$lnP^o = \frac{B}{T} + A$$

$$B = \left(\frac{\Delta H_{12}}{R}\right)$$

which represents a linear relationship between the partial pressure and temperature.

Changing notation for land- and water-based source, we have:

$$lnP^{oL} = -\frac{B_L}{T^L} + A_L \qquad lnP^{oW} = -\frac{B_W}{T^W} + A_W$$

$$B_L = \left(\frac{\Delta H_{12}^L}{R}\right) \qquad B_W = \left(\frac{\Delta H_{12}^W}{R}\right)$$

This brief report summarizes my thoughts on a possible procedure that utilizes the available data in such a way as to increase the accuracy of temporal and spatial estimates of PCB concentrations over and around Lake Michigan.

Appendices

Appendix A
Lake Michigan Mass Balance Project: Modeling Work Plan

Issue Identification

The Laurentian Great Lakes have proven highly susceptible to the effects of anthropogenic pollutants including nutrients and toxic chemicals. Persistent toxic chemicals, such as PCBs, remain a threat to human and ecosystem health in the Great Lakes, despite decade-old limitations on their production and use. Other toxics, such as mercury and current-use pesticides, continue to accumulate in the Great Lakes due to non-point sources. In the Great Lakes basin, nearshore sediment contamination by persistent toxics is widespread: all of the 42 Areas of Concern designated by the IJC suffer impairments from contaminated sediments. In the lakes themselves, the problem of contaminated sediments is compounded by the deposition of persistent toxic chemicals from near-field and regional-scale atmospheric transport. Biomagnification of toxics through the aquatic food web results in concentrations in top predator fish which exceed consumption guidelines, and greatly exceed more stringent, risk-based criteria. As a consequence, reproductive failure and deformities of fish and fish-consuming wildlife are reported, commercial and recreational fisheries are closed or limited by consumption advisories, and other impacts including developmental retardation in children of sports fishermen have been documented (Environment Canada, 1991). Although actions taken to control bioaccumulative toxics were initially effective in reducing contaminant concentrations in the Great Lakes, such trends have generally not been observed in recent years. Understanding the sources, transport pathways, fate, and bioaccumulation of persistent toxic chemicals is essential to allow development of effective remedial action plans and load reduction efforts to further reduce contaminant concentrations in the ecosystem. While considerable progress has been made in understanding the cycling of toxics in the Great Lakes ecosystems, there is still a lack of quantitative information from which to forecast the effectiveness of toxics management alternatives.

In response to these issues, efforts to control toxic chemicals on a lake-wide basis are being developed for each of the Great Lakes. The USEPA, GLNPO has proposed a mass balance approach to develop a LaMP to address toxics in Lake Michigan (USEPA, 1995a). The LMMBP will also study hazardous air pollutants for the CAAA's Great Waters Program. The mass balance approach, demonstrated in the GBMBS, provides a consistent framework for integrating load estimates, ambient monitoring data, process research efforts, and modeling, leading to the development of scientifically credible, predictive cause-effect tools. The primary goal of the mass balance study is to develop a sound, scientific base of information to guide future toxics load reduction efforts for Lake Michigan at the state and federal levels. From this goal, a number of specific objectives have been identified. Several of the plan's objectives call for identifying and quantifying the sources of toxics to Lake Michigan, as well as establishing cause-effect relationships and developing forecasting tools:

1. Determine loading rates for critical pollutants from major source categories (tributaries, atmospheric

deposition, contaminated sediments) to establish a baseline loading estimate to gauge future progress, and to better target future load reduction efforts.

2. Predict the environmental benefits (in terms of reducing concentrations) of specific load reduction alternatives for toxic substances, including the time required to realize the benefits.

3. Evaluate the environmental benefits of load reductions for toxic substances expected under existing statutes and regulations and, thereby, determine if there is a need for more stringent, future regulations to realize further benefits.

4. Improve our understanding of how key environmental processes govern the transport, fate, and bioavailability of toxic substances in the ecosystem.

The mass balance project will be based upon the Enhanced Monitoring Program (EMP), a comprehensive, two-year synoptic survey for selected toxic chemicals in the Lake Michigan ecosystem. The EMP will include tributary load and atmospheric deposition monitoring; ambient water column, biota, and sediment sampling; and additional measurements to define and confirm transport and fate processes. In support of the mass balance study, the USEPA, ORD, NHEERL, MED-Duluth, CBSSS at the LLRS, Grosse Ile, Michigan, in cooperation with the ORD, Atmospheric Research and Exposure Assessment Laboratory (AREAL), the NOAA-GLERL, and other cooperators, will develop a suite of integrated mass balance models to simulate the transport, fate and bioaccumulation of toxic chemicals in Lake Michigan. This work plan describes these models, the manner in which they will be integrated, the relationship between their development and the EMP data, and their intended application.

This project directly supports the development of a LaMP for Lake Michigan, mandated under Section 118 of the 1992 Clean Water Act (CWA) as well as Annex 2 of the GLWQA, and a study for the Great Waters Program mandated by Title III, Section 112(m) of the CAAA-90. USEPA also intends the LaMP to serve as the basis for development and submission of State Water Quality Management Plans developed in accordance with Sections 208 and 303(b) of the CWA, as implemented through 40 CFR 130.6.

Modeling Purpose and Objectives: Mass Balance Approach

Development of effective strategies for toxics management requires a quantitative understanding of the relationships between sources, inventories, concentrations, and effects of contaminants in the ecosystem. A mass balance modeling approach is proposed in this work plan, to address the relationship between sources of toxic chemicals and concentrations in air, water, sediment, and biota. This approach integrates load estimation, ambient monitoring and research efforts within a modeling framework that is compatible with both scientific as well as ecosystem management objectives. The mass balance approach estimates the magnitude of mass fluxes that constitute the pathways for toxics transport into and out of the lake, that distribute toxics within the lake water column and sediment, and that lead to bioaccumulation of the aquatic food web. Based upon these estimates, the mass balance can determine the rate of change in concentrations and inventories of toxics as inputs such as atmospheric and tributary loadings are changed, or other aspects of the system are perturbed. Thus, the mass balance can serve as a useful tool to estimate or predict the outcome of alternatives under consideration for toxics management.

More specifically, the modeling efforts associated with the LMMBP will meet the following objectives:

1. Provide a consistent framework for integrating load estimates, ambient monitoring data, process research efforts, and prior modeling efforts, leading to a better understanding of toxic chemical sources, transport, fate and bioaccumulation in Lake Michigan.

2. Estimate the loading of priority toxics, solids, and nutrients from all major tributaries to Lake Michigan for the duration of the EMP study.

3. Estimate the atmospheric deposition and air-water exchange of priority toxics, including spatial and temporal variability over Lake Michigan.

4. Calibrate and confirm mass balance models for priority toxics using EMP data, based upon models for hydrodynamic and sediment transport, eutrophication/organic carbon dynamics, toxics transport and fate, and food web bioaccumulation.

5. Based upon the mass balance models, evaluate the magnitude and variability of toxic chemical fluxes within and between lake compartments, especially between the sediment and water column and between the water column and the atmosphere.

6. Apply the mass balance models to forecast contaminant concentrations in water and sediment throughout Lake Michigan, based upon meteorological forcing functions and future loadings based upon load reduction alternatives.

7. Predict the bioaccumulation of persistent toxic chemicals through the food web leading to top predator fish (lake trout and coho salmon) for specific fish populations in the lake, in order to relate mass balance predictions of water and sediment exposure to this significant impaired use.

8. Estimate (quantify) the uncertainty associated with estimates of tributary and atmospheric loads of priority toxics, and model predictions of contaminant concentrations.

9. Identify and prioritize further monitoring, modeling, and research efforts to (1) address additional toxic substances, (2) further reduce uncertainty of predictions, (3) establish additional cause-effect linkages, such as ecological risk endpoints and feedbacks, and (4) evaluate additional source categories, such as non-point sources in the watershed.

The purpose of modeling will be to simulate the transport, fate and bioaccumulation of four priority toxics in Lake Michigan: PCB congeners, TNC, atrazine, and total mercury. These toxics are collectively referred to as "contaminants" in this work plan. Rationale for the selection of these contaminants is presented in the Mass Balance Project work plan, and briefly reviewed here:

PCBs are a group of persistent, bioaccumulative hydrophobic organic chemicals (HOCs) that are ubiquitous in the Great Lakes. Although anthropogenic inputs from production and disposal largely ceased following their ban in the 1970s, atmospheric and watershed/tributary transport pathways to the lake continue the import of PCBs. In addition, a large in-lake sediment inventory represents an internal source of PCBs, which are recycled annually. PCBs have been consistently identified as the contaminants of greatest concern to human and ecosystem health the Great Lakes (Ludwig *et al*., 1993; Gilbertson, 1988).

TNC is a bioaccumulative chlordane, representative of cyclodiene insecticides used in the 1970s. Like PCBs, TNC is bioaccumulative and concentrations in Lake Michigan fish exceed consumption guidelines.

Atrazine is a current-use herbicide in wide use throughout the Great Lakes basin. It is reactive, undergoing several biotic and abiotic transformations in soil; little is known about its fate in receiving waters such as the Great Lakes. Atrazine is soluble relative to the other mass balance contaminants, therefore, partitioning and bioconcentration should be relatively insignificant.

Mercury is a metal which, in its methylated form, is bioaccumulative and toxic. Mercury concentrations have reportedly increased in surface waters, including the Everglades and inland lakes of the Midwest, but apparently not in the Great Lakes. Mercury concentrations in fish exceed consumption guidelines, for some species and locations in the Great Lakes. Concern that increasing atmospheric emissions, from sources such as coal-fired power generation and waste incineration, will lead to increased atmospheric deposition to the Great Lakes also motivates inclusion of mercury in this mass balance effort.

Background - Prior Modeling Efforts

The modeling design and approach for the LMMBP reflects a progression of prior modeling efforts, in Lake Michigan and throughout the Great Lakes. These include eutrophication and toxic substance mass balance models, food web bioaccumulation models, and predictive hydrodynamic and sediment transport models. Although not a comprehensive review, several of these prior modeling efforts are discussed below:

Lake-1 A eutrophication model for Lake Michigan was developed by Rodgers and Salisbury (1981), based upon the Lake-1 model which was also applied in Lakes Erie, Huron, and Ontario. The model was calibrated and tested using data from 1976 and 1977. The importance of climatic factors on limnological (including eutrophication)

processes in Lake Michigan was demonstrated, as the severe winter and extensive ice cover of 1976-77 dramatically reduced total phosphorus concentrations in the second year. This work also identified several refinements necessary for accurate modeling of eutrophication: phosphorus availability to phytoplankton and particle transport including shoreline erosion and sediment resuspension were apparently significant influences upon nutrient and phytoplankton dynamics observed in Lake Michigan.

Completely Mixed Lake A lakes-in-series model for conservative substances was developed by Sonzogni *et al*. (1983), and applied to forecast chloride concentrations in each of the Great Lakes as a function of expected future loadings. This model demonstrated that concentrations of non-reactive substances would substantially "lag" the history of their input. This was especially the case for Lake Michigan, where maximum chloride concentrations were not predicted to occur until the 22nd century despite declining loads after the 1970s. Similarly strong, non-steady-state behavior may be expected for other chemicals which are non-reactive and weakly associated to particles.

General Mass Balance Framework for Toxic Chemicals in the Great Lakes At about the same time, models were being developed which would serve as the foundation for describing and simulating the transport and fate of hydrophobic chemicals in the Great Lakes. Thomann and Di Toro (1983) and Robbins (1985) demonstrated that the lake-wide, annual concentration trend of contaminants including cesium-137, plutonium-239/240, and PCBs, were dependent upon particle transport between the water column and a resuspendable sediment compartment. The principal loss mechanisms from the lakes were found to be burial by sedimentation and (for PCBs) volatilization. The somewhat paradoxical behavior of these models, was that the water column contaminant dynamics were largely controlled by sediment parameters.

Food Web Bioaccumulation Model A food web bioaccumulation model was developed by Connolly and Thomann (1985) and applied to simulate bioaccumulation of PCBs in Lake Michigan lake trout. The model was confirmed with an extensive data set collected in 1971, including nine age classes of trout, diet characterization by gut contents analysis, and alewife. The model was successful in predicting bioaccumulation for mature age classes of lake trout, although not for juveniles. Dietary transfer was demonstrated to be the predominant route of PCB accumulation, in comparison to direct chemical uptake from water. Substantial residual variance in lake trout PCB concentrations (within age class CV $\approx$ 1) was not explained by this lake-wide, average-individual model.

MICHTOX An integrated mass balance and bioaccumulation model for PCBs and 10 other toxic chemicals was developed as a planning tool for the LMMBP (Endicott *et al*., 1992). The MICHTOX mass balance was calibrated to suspended solids and plutonium data for the southern lake basin, while the bioaccumulation model combined Connolly and Thomann's effort with chemical-specific parameterization from Lake Ontario. MICHTOX demonstrated that reasonable predictions of PCB concentration trends in water, sediment and biota could be developed; although significant uncertainties regarding sediment-water and air-water contaminant transport remain. These are the most significant transport fluxes for PCBs (as illustrated by predicted annual PCB fluxes, Figure 1) and presumably other hydrophobic contaminants. Major data gaps for other priority toxics allowed only order-of-magnitude estimates of load-concentration relationships. Available monitoring data for toxic chemical concentrations in tributaries, air, lake water, sediment, and biota are not adequate to define loading trends in the last decade, or to relate the distribution of loadings to contaminant gradients observed for sediment and biota. Credible model predictions of toxic chemical transport, fate, and bioaccumulation would depend upon developing a comprehensive data set quantifying loadings, sediment inventories, concentrations and transport fluxes on a spatially-resolved basis, and localized descriptions of food web structures.

Green Bay Mass Balance Study This study demonstrated the feasibility of applying mass balance principles to manage toxic chemicals in the Great Lakes ecosystem. A two-year (1989-1990) synoptic sampling program was designed to collect appropriate and complete data for the mass balance study. A suite of integrated mass balance and bioaccumulation models were developed, which together, provide an ecosystem-level simulation of sources, transport, fate, and bioaccumulation of PCBs throughout the Fox River and Green Bay. This study advanced the state-of-the-art of mass balance modeling, particularly the ability to construct a fairly complete and accurate description of contaminant mass transport.

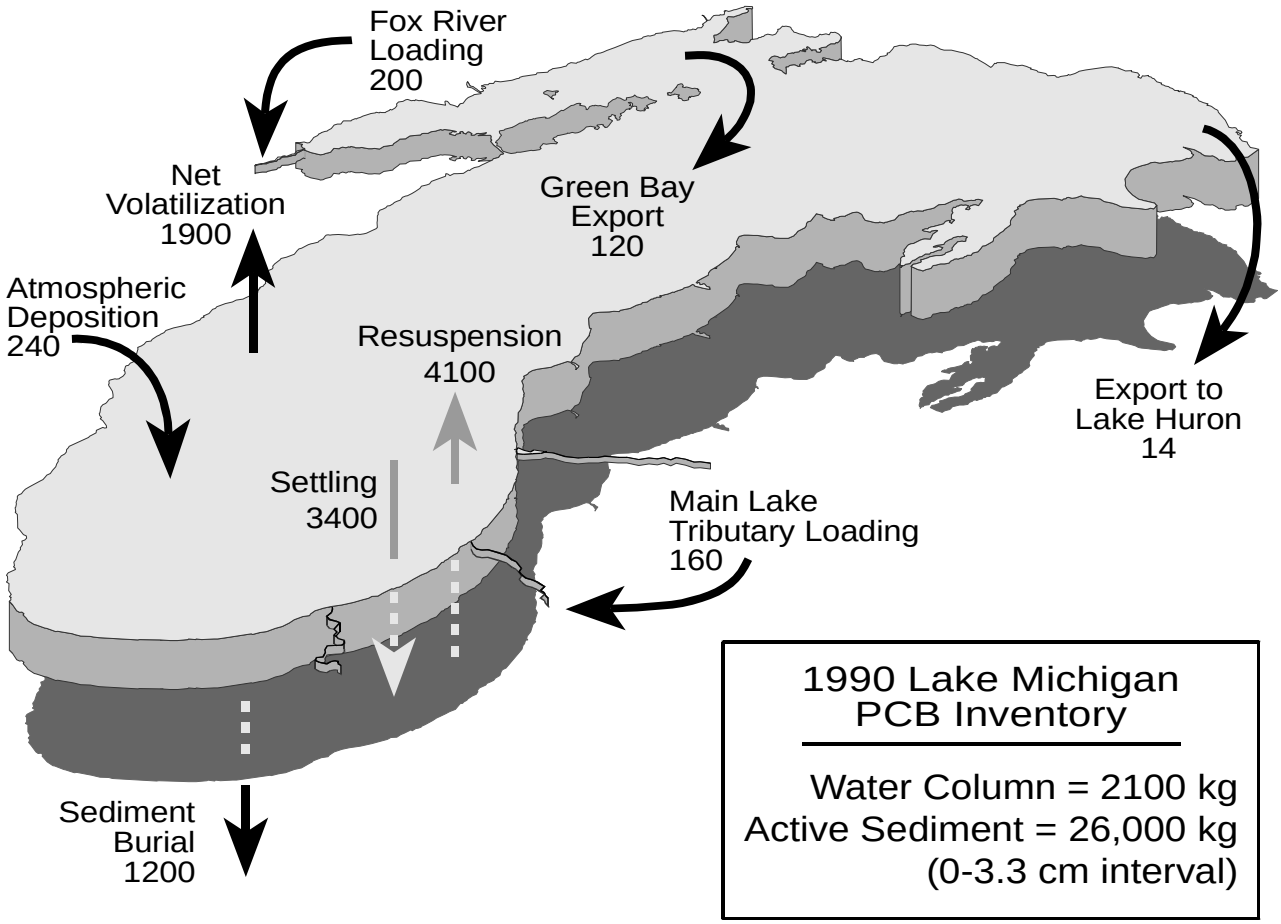


Figure 1. 1990 MICHTOX estimates of PCB fluxes (PCB fluxes in kg).

Several aspects of the Green Bay modeling effort were noteworthy. Particle transport and sorption processes were found to be of fundamental importance as bases for contaminant modeling. Resuspension of contaminated sediments in the Fox River constituted the major source of PCBs to the river as well as the bay. In the bay, particle sorbent dynamics were strongly affected by phytoplankton production and decay. The relative significance of hydraulic and sediment transport, burial, volatilization, and open lake boundary exchange processes upon the PCB mass balance, varied considerably with location in Green Bay. Radionuclide tracers were again essential for calibration of particle fluxes and confirmation of long-term contaminant transport predictions. The significance of contaminant accumulation at the base of the food web, and fish movement in relation to exposure gradients, were demonstrated in the bioaccumulation model. The mass balance study demonstrated the linked submodel approach to ecosystem model development and application, and the feasibility of using such a model for assessing the effectiveness of toxics management control alternatives.

SEDZL The GBMBS also provided data to test a predictive two-dimensional, hydrodynamic and sediment transport model of the Fox River, SEDZL (USEPA, 1995b). SEDZL incorporates realistic descriptions of cohesive sediment resuspension, flocculation and deposition processes, and contaminant sorption, which are

critical for accurate prediction of hydrophobic contaminant transport. These process descriptions are based on laboratory and field experiments with river, bay, and lake sediments. A three-dimensional bed sub-model is used to describe sediment bed properties which vary with depth as well as location. The fine spatial resolution of the model allows detailed simulation of in-place pollutant transport in both the water column and sediment bed. Although computationally intensive and requiring specialized data, SEDZL has substantially advanced the state-of-the-art for sediment and contaminant transport modeling in the Great Lakes. SEDZL has also been applied to the Buffalo and Saginaw Rivers as part of the ARCS/RAM project (Gailani *et al*., 1994; Cardenas and Lick 1996). These applications included long-term forecasts (10-25 years) of sediment and contaminant transport. SEDZL has also been applied to large water bodies such as Lake Erie, and marine coastal waters including Santa Barbara Channel, and Atchafalaya Bay where wave action as well as currents force sediment resuspension. A three-dimensional version of SEDZL is being tested currently on Green Bay.

Modeling Framework

The model design for the LMMBP is based upon the linked sub-model approach used in the GBMBS, and retains the same basic models: hydrodynamics, sediment transport, sediment bed dynamics, eutrophication/ sorbent dynamics, contaminant transport and fate, and food web bioaccumulation. A schematic representation of the overall mass balance design is shown in Figure 2. The Lake Michigan submodels will be applied at several different levels of resolution, and will incorporate predictive hydrodynamic and sediment transport simulations as the modeling "foundation". This approach is consistent with other state-of-the-art ecosystem modeling exercises, such as the Chesapeake Bay Watershed Model (Linker *et al*., 1993), which emphasize increasing computational effort, complexity, and predictive resolution. As discussed below, linkages will also be established with atmospheric transport and watershed delivery models, to allow simulation of multimedia toxics transport as well as loads and boundary conditions to the lake. Ultimately, such linkages will be essential to relate watershed and "airshed" management to water quality. Descriptions of the lake process, atmospheric and watershed delivery model frameworks follow.

Lake Process Models

The mass balance for toxics in Lake Michigan will be comprised of linked hydrodynamic, eutrophication/sorbent dynamics, particle transport, contaminant transport and transformation, and bioaccumulation simulations. Each of these models represents significant processes affecting the mass balance for toxic chemicals. The hydrodynamic model predicts water movements necessary to describe the three-dimensional transport of dissolved and particulate constituents in the water column. The eutrophication model describes the production, respiration, grazing and decomposition of planktonic biomass within the lake. The particle transport model describes the resuspension, transport and deposition of particulate materials including sorbent phases necessary to describe the movement of particle-associated contaminants. The contaminant transport and fate model describes contaminant partitioning between dissolved and sorbed phases, transfer between media (air, water, sediment), and biogeochemical transformations. The bioaccumulation model simulates contaminant accumulation from water and sediments to predator fish via direct exposure and trophic transfer through benthic and pelagic food webs. Together, these submodels form an integrated description of toxic chemical cycling in the aquatic ecosystem, with which to predict the relationship between loadings and concentrations for contaminants of interest.

A. Hydrodynamics

The Princeton Ocean Model (POM; Blumberg and Mellor, 1987) will be used to compute three-dimensional current fields in the lake. The POM will simulate large- and medium(km)-scale circulation patterns, vertical stratification and velocity distribution, seiche, and surface waves. This model will also be used to simulate a thermal balance for the lake, and will generate turbulent shear stresses for the sediment transport model. The POM is a primitive equation, numerical hydrodynamic circulation model that predicts three-dimensional water column transport in response to wind stress, temperature, barometric pressure, and Coriolis force. The POM has been demonstrated to accurately simulate the predominant physics of large water bodies (Blumberg and Mellor, 1987). This model will be used to develop year-long simulations on a 5 km horizontal grid, with 15 sigma-coordinate vertical levels, at one-hour intervals for

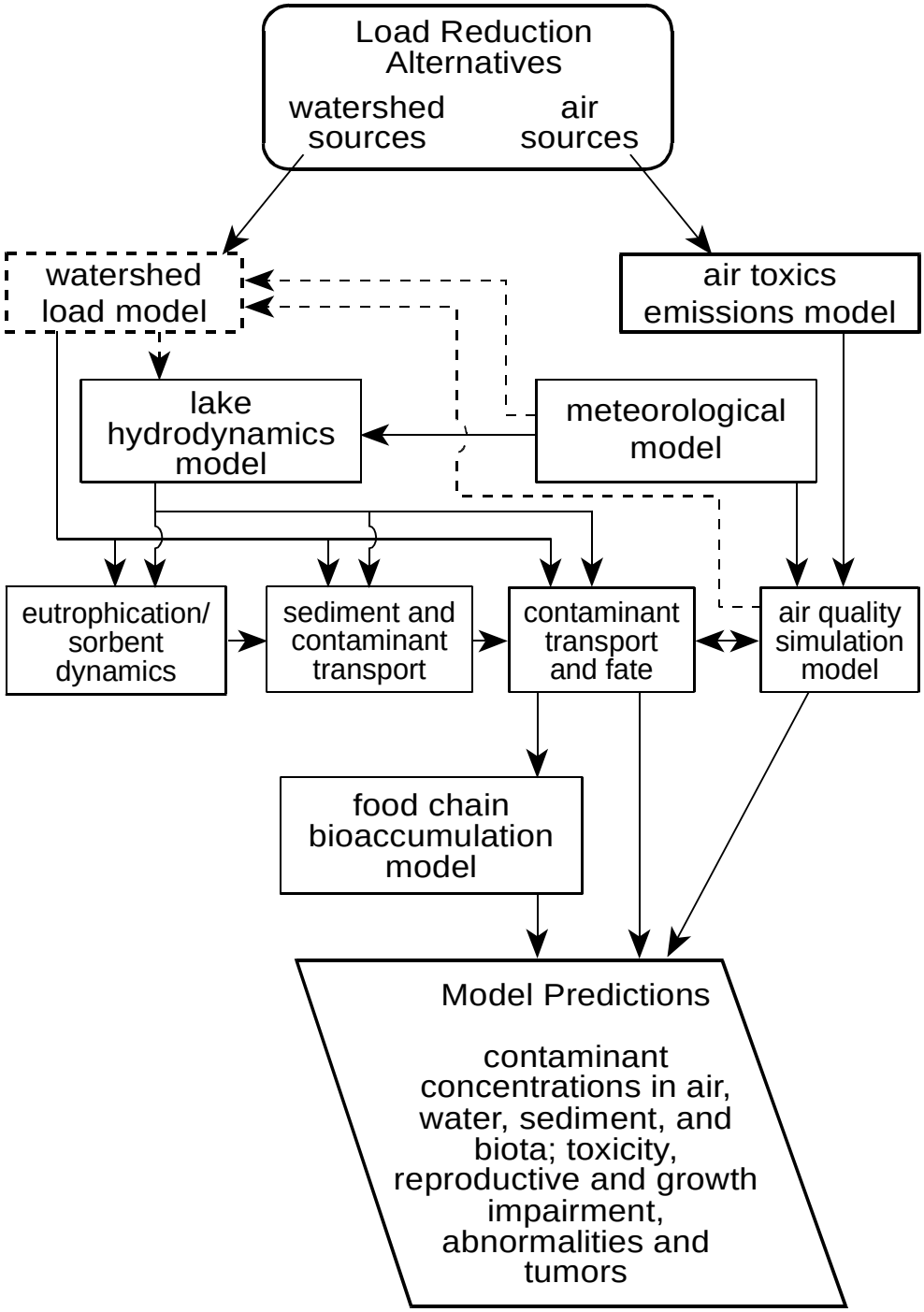


Figure 2. Integrated submodel design for Lake Michigan mass balance project.

Lake Michigan. Observed and simulated meteorological data will be used to define model forcing functions. Extensive measurements of temperature, transmissivity, and current distributions collected in Lake Michigan during 1982-1983 will provide the necessary data for model confirmation; measurements of daily surface temperature (from satellite) and temperature, transmissivity, and current distributions will also be used to confirm hydrodynamic simulations for 1994-1995.

The hydrodynamic model is the appropriate transport foundation for an accurate lake mass balance model, for a number of reasons. A confirmed hydrodynamic model offers a credible basis for extrapolating transport, in terms of forecasting the response to expected and extreme meteorological forcing functions, that is desirable for a mass balance simulation. The hydrodynamic model results are scalable to provide transport predictions at the desired spatial and temporal resolution. This is useful when considering that the various processes incorporated in the mass balance are not necessarily modeled at the same scale or resolution, yet all depend upon a consistent transport simulation. In particular, the sediment and contaminant transport model described below, requires high resolution simulations of current- and wave-induced shear stress to predict sediment transport. Hydrodynamic models are also transportable, with little system-specific parameterization in comparison to traditional water quality models. A mass balance design based upon hydrodynamic transport is advantageous, for instance, when considering transporting the mass balance model from Lake Michigan to the other Great Lakes.

B. Sediment and Contaminant Transport

A three-dimensional version of the sediment transport model, SEDZL, will be used to simulate the movement of sediment particles in both the water column and sediment bed, including settling, resuspension, flocculation, transport and deposition. SEDZL will simulate the significant short- and long-term processes which transport sediment particles and particle-associated contaminants in the lake. SEDZL will be linked to hydrodynamic output from the POM, and will be based upon the same three-dimensional water column grid. State variables will include three particle classes (plankton/biotic solids, cohesive fine-grained sediment/detritus, and coarse-grained solids) and PCBs. SEDZL will simulate the 1982-1983 and 1994-1995 periods for which hydrodynamic forecasts will be available, as well as intensive confirmation data provided by sediment trap and radionuclide monitoring. Further confirmation data for 1994-95 will be provided by remote sensing, transmissometer arrays, and water intake monitoring. Sediment bed properties, particle resuspension rate parameters, flocculation parameters and settling properties necessary for the model will be determined by field measurements to be performed on Lake Michigan sediments, and by results of experiments conducted with other sediments from the Great Lakes. Allochthonous sediment loadings will be estimated for tributary export, shoreline erosion, and atmospheric particle deposition. Autochthonous production will be provided from the eutrophication/sorbent dynamics model, and input as loadings to the sediment transport model.

The sediment transport model is applied to predict the transport of particles in the lake, which predominantly carry hydrophobic contaminants for near-shore locations such as tributary mouths, to deposition zones usually in deep water. The transport of sediment and associated contaminants is a complex interaction of the properties of sediment particles and the sediment bed, circulation, bathymetry, and turbulent shear stresses applied by waves and current. Moving from shore to deep water, regimes of sediment transport are encountered, resulting in distinct distributions of grain size, bed thickness, sedimentation rate, and contaminant concentrations in the lake sediments. Contaminants move along this gradient associated primarily with the fine-grained sediments, yet their transport is influenced by the entire particle assemblage. In terms of resuspension and deposition, most sediment transport is associated with the sequence of short, infrequent events such as storms. SEDZL simulates the interactions and dynamics of sediment transport, and offers predictive capabilities beyond that obtainable by a calibrated-transport approach. Advantages include compatibility with the hydrodynamic simulation, high spatial resolution consistent with the spatial variability of the resuspension process, and verified process descriptions for the dynamics of sediment

resuspension and deposition under event conditions which are the most difficult to model. SEDZL predictions have been confirmed mostly in tributary systems; in large water bodies simulations have been conducted for events, with only limited confirmation. Thus, significant development is still required for credible application of SEDZL in the Lake Michigan mass balance model. Sediment and contaminant transport model predictions will require extensive confirmation against EMP data to ensure model credibility.

The alternative approach to treating sediment transport is descriptive, where direct calibration of total suspended solids and associated particle tracers is used to specify settling and resuspension fluxes. The descriptive approach ensures a model calibration that is consistent with available observations. However, the spatial complexity and event-responsive nature of sediment transport described above introduce too many degrees of freedom to allow model calibration to the data being generated by the EMP. This approach relies entirely upon fitting suspended constituent data, which will be too sparse (both in space and time) to allow accurate description of sediment transport fluxes. The second major disadvantage of descriptive transport, is that the resulting model has no forecasting basis other than replaying the calibration. Attempts to go beyond the calibration are, in general, weak emulations of predictive transport approaches.

C. Eutrophication/Sorbent Dynamics

The eutrophication/sorbent dynamics (ESD) model predicts the production, transformation and decay of plankton biomass in response to seasonal dynamics of temperature, light, and nutrient concentrations. In the open lake, living and dead plankton comprise the majority of suspended particles and generate significant autochthonous loads of particulate and dissolved organic carbon (POC and DOC) to which PCBs and other contaminants preferentially partition (Richardson *et al*., 1983; DePinto *et al*., 1993). The ESD model simulates the non-conservative, seasonally-variable dynamics of the biotic organic carbon pool, which has a significant influence upon partitioning of HOCs (Dean *et al*., 1993). Such a model was applied to simulate the dynamics of organic carbon states in Green Bay as part of the GBMBS (DePinto *et al*., 1993). However, a more resolute, multi-class eutrophication model (Bierman and McIlroy, 1986) will be applied to Lake Michigan, and the linkage between plankton and organic carbon states will be refined. Model outputs include autochthonous solids loads, and transformation and decay rates, that will be used as inputs for the sediment transport and the contaminant transport and fate models. The biomass growth rates may also be linked to the plankton bioconcentration submodel of the food web bioaccumulation model.

The ESD model is an important component of the mass balance model for hydrophobic contaminants, because it simulates the dynamics of a significant sorbent particle class (phytoplankton) in the water column. The dynamics of phytoplankton production and loss cannot be adequately described by seasonal EMP limnological monitoring, which will occur too infrequently to observe major events such as blooms, assemblage shifts, and die-offs. Furthermore, the ESD model component will allow forecasting for integrated toxics and nutrient management options, because mass balances for toxics and nutrients are coupled via eutrophication/sorbent dynamics processes. Finally, the ESD model is the appropriate framework for inclusion of zebra mussels in the mass balance model. Zebra mussels, which at high density can impact the lower food web and alter sediment and contaminant transport, are currently (1994) infesting Lake Michigan and are reaching high densities in suitable locations such as Green Bay.

D. Contaminant Transport and Fate

The mass balance for toxic chemicals in the lake will be computed in a contaminant transport and fate (CTF) model which describes contaminant transport, intermedia exchange, phase distribution, and biogeochemical transformations, in both the water column and sediments. The CTF model will be calibrated and confirmed for each of the priority toxics: atrazine, mercury, selected individual and sum of PCB congeners, and TNC. Mass balance analyses will be performed for each contaminant, to evaluate the significant source, transport, and loss pathways. Effectiveness of alternative load reduction scenarios upon reducing toxic chemical concentrations, will also

be forecast. Although calibration and confirmation will be limited to the period of available EMP data, the CTF model will be required to forecast contaminant concentrations for substantially longer periods: on the order of 20-50 years. Long simulations are necessary because of the substantial lag time associated with the chemical concentration response in the lake to changing loads. The lag time is associated with the residence time of contaminants in the surficial sediments, which is constrained by confirmation of CTF model hindcasts for cesium-137 and/or plutonium-239/240. These particle-associated radionuclides have been demonstrated as important tracers for the long-term transport of sediments and contaminants in Lake Michigan and the Great Lakes. Because their loading histories are known with relative certainty, available water and sediment data for these contaminants are directly useful for model confirmation. Such data are critical to develop of a model intended to make long-term forecasts, especially since EMP monitoring will be only two years in duration. Intensive sediment trap data collected in 1982-1983 (Robbins and Eadie, 1991) and water column measurements from the same period, will provide further measurements for confirmation of particle transport fluxes.

A schematic diagram of the CTF model as applied for PCBs in Lake Michigan is presented in Figure 3. Chemical fluxes between model compartments are computed from advective and dispersive transport of aqueous and particulate contaminant fractions. The model will describe chemical partitioning between dissolved and particulate sorbent compartments, including multiple particle types, using an organic carbon-based equilibrium assumption. Both local equilibrium and first-order kinetic partitioning process descriptions will be tested. Chemical transformations such as hydrolysis and biodegradation are modeled as first-order or pseudo first-order reactions, with daughter chemicals retained in the mass balance as additional state variables (for atrazine, these include diethylatrazine and deisopropylatrazine). For mercury, a two-state (organic and inorganic) multiple-sorbent class framework proposed by Thomann (1993) will be applied.

The CTF model incorporates simulations of other submodels (Figure 2) by the following linkages:

Submodel	Data Linkage
POM/SEDZL	Hydrodynamic and sediment transport; water temperature
Eutrophication/ sorbentdynamics	Autochthonous load; transformation and decay rates
Meteorological model	Wind and air temperature
Atmospheric model	Boundary conditions and fluxes
Watershed delivery model	Tributary loads

The CTF model will be linked to hydrodynamic and sediment transport simulations, by appropriate filtering and averaging of transport fields (Hamrick, 1993; Dortch *et al*., 1992). Total suspended solids and $\sum$PCB (sum of congeners) simulations will be reproduced in both SEDZL and CTF models, providing computational "tracers" to validate the transport linkages.

The CTF model will be applied at an intermediate (Level 2) scale. In the water column, segment resolution is defined at a scale compatible with the definition of food web zones (approximately 20 x 40 km), with 2-5 vertical layers. In sediments, segmentation will be based upon discretization of deposition regime and contaminant distribution, with 1 cm vertical resolution. Fine-scale simulations are necessary for accurate predictions of hydrodynamic and cohesive particle transport as well as accurate simulation of short-duration event processes. However, the computational cost of fine-scale models is high and makes long-term (20 to 30 year) simulations infeasible, especially with the significant number of state variables required for multiple contaminants, sorbent phases, etc. Resolution at the scale of POM and SEDZL is also not appropriate for the mass balance objectives of this project. Intermediate scale models have substantially lower computational cost and have been demonstrated for contaminant transport and transformation over temporal and spatial scales appropriate for toxics

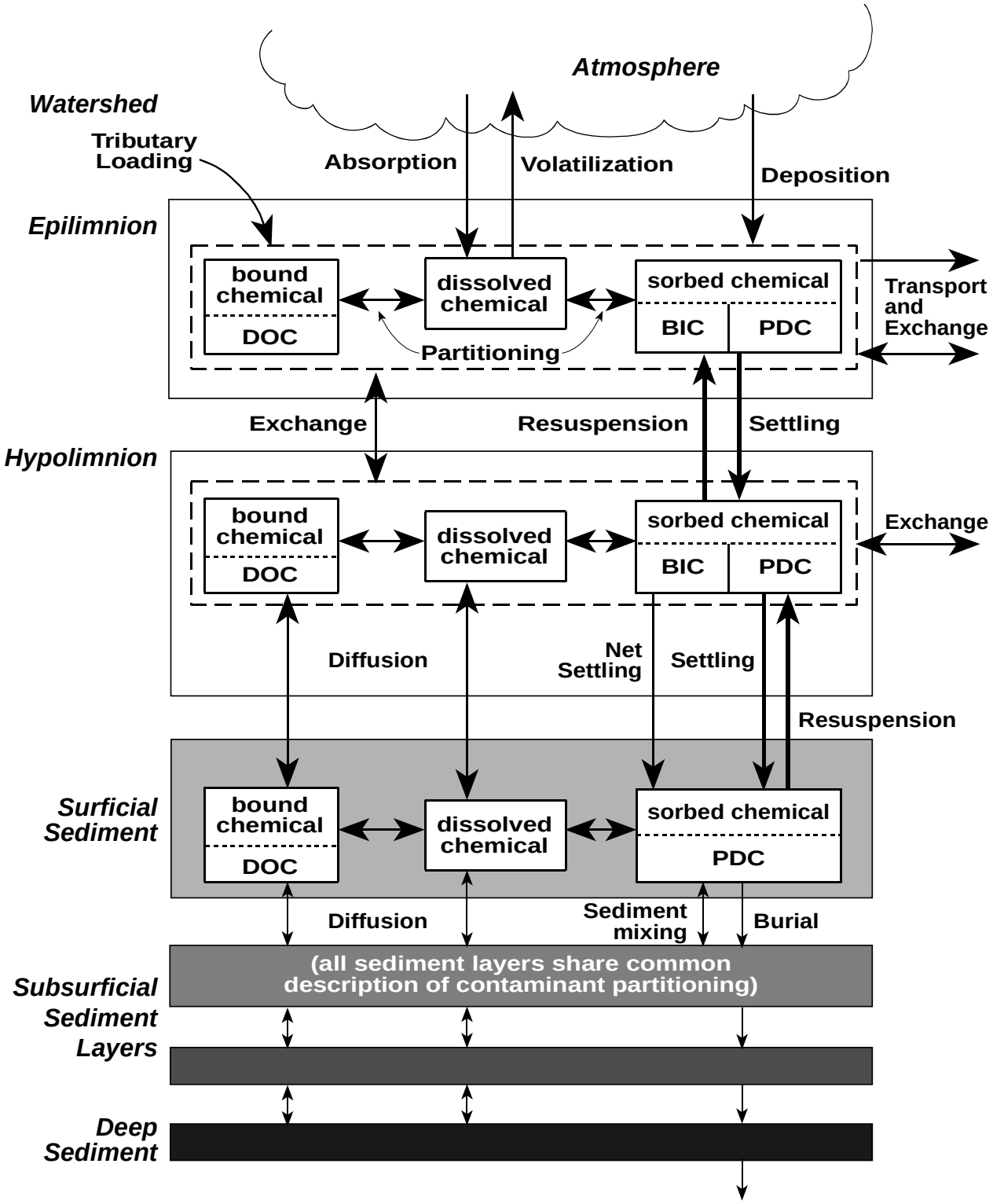


Figure 3. Contaminant transport and fate model schematic.

exposure prediction and linkage to bioaccumulation models (DePinto *et al*., 1993; Connolly *et al*., 1992).

Although CTF model descriptions are generally well-defined, no single framework presently available has the capacity to accurately predict all components of CTF while retaining the aggregate behavior of hydrodynamic and sediment transport simulations. To develop an appropriate framework for the LMMBP and future lake-wide analysis and management projects, existing and developmental mass balance water quality modeling frameworks such as those used for Chesapeake Bay (Cerco and Cole, 1993), Green Bay (Bierman *et al*., 1992; Velleux *et al*., 1994), and other projects (Richards, 1990; Katopodes, 1994) will be reviewed. Appropriate features of these models will be synthesized into a single framework and extended to meet the requirements of the LMMBP.

D. Food Web Bioaccumulation

A bioaccumulation model simulates chemical accumulation in the food web in response to chemical exposure, based upon chemical mass balances for aquatic biota. The general form of the bioaccumulation equation is well defined, and equates the rate of change in chemical concentration within a fish (or other aquatic organism) to the sum of chemical fluxes into and out of the animal. These fluxes include direct uptake of chemical from water, the flux of chemical into the animal through feeding, and the loss of chemical due to elimination (desorption and excretion) and dilution due to growth. To predict bioaccumulation for top predator fish (the modeling objective here), the bioaccumulation mass balance is repeatedly applied to animals at each trophic level to simulate chemical biomagnification from primary and secondary producers, through forage species to top predators. Food web bioaccumulation models have been successfully applied for PCBs and other HOCs in several large-scale aquatic ecosystems (Thomann and Connolly, 1984; Connolly and Tonelli, 1985) and, most recently, for the GBMBS (Connolly *et al*.,1992). The model developed for that project, FDCHN, will be adapted for use in Lake Michigan. FDCHN is a time-variable, population-based age class model, incorporating realistic descriptions of bioenergetic, trophodynamic, and toxicokinetic processes. The general features of FDCHN are well-suited to a modeling application such as the LMMBP.

For Lake Michigan, bioaccumulation of PCB congeners and TNC will be modeled for lake trout and coho salmon food webs. Food web bioaccumulation will be simulated for sub-populations of lake trout in three distinct biotic zones. The general structure of the lake trout food web in Lake Michigan is shown in Figure 4. In each zone, different food webs support lake trout, including benthic and pelagic food web linkages. Biotic zones are defined by the approximately 50-mile range of movement of lake trout. The coho salmon, in comparison, is strictly pelagic. Although the coho food web is simpler, the bioaccumulation simulation must account for significant migration over the two year lifetime of this stocked salmonid in Lake Michigan.

It should be recognized that FDCHN, and in fact, all current food web bioaccumulation models, is not predictive in terms of the dynamics of the food web itself. In other words, the food web structure is described as model input. FDCHN does not predict changing forage composition, trophic status in response to nutrients, exotic species invasion, or fisheries management. Yet such factors have been demonstrated to alter food web structures in the Great Lakes, and these changes have been suggested to affect bioaccumulation in top predators including salmonids.

To address the sensitivity of bioaccumulation predictions to food web dynamics, the SIMPLE model (Jones *et al*., 1993), a bioenergetic model for fish population dynamics in the Great Lakes, will be used to construct scenarios for food web change that will then be tested in FDCHN. While less satisfactory than an integrated population dynamics simulation, such testing will demonstrate the sensitivity of bioaccumulation predictions to food web dynamics in comparison to changes in contaminant concentrations in fish due to reducing exposure concentrations.

Atrazine bioaccumulation will not be modeled, because it is not expected to accumulate in biota due to its low hydrophobicity. It is not presently feasible to model bioaccumulation of mercury because a mass balance for the bioaccumulative fraction (the methyl

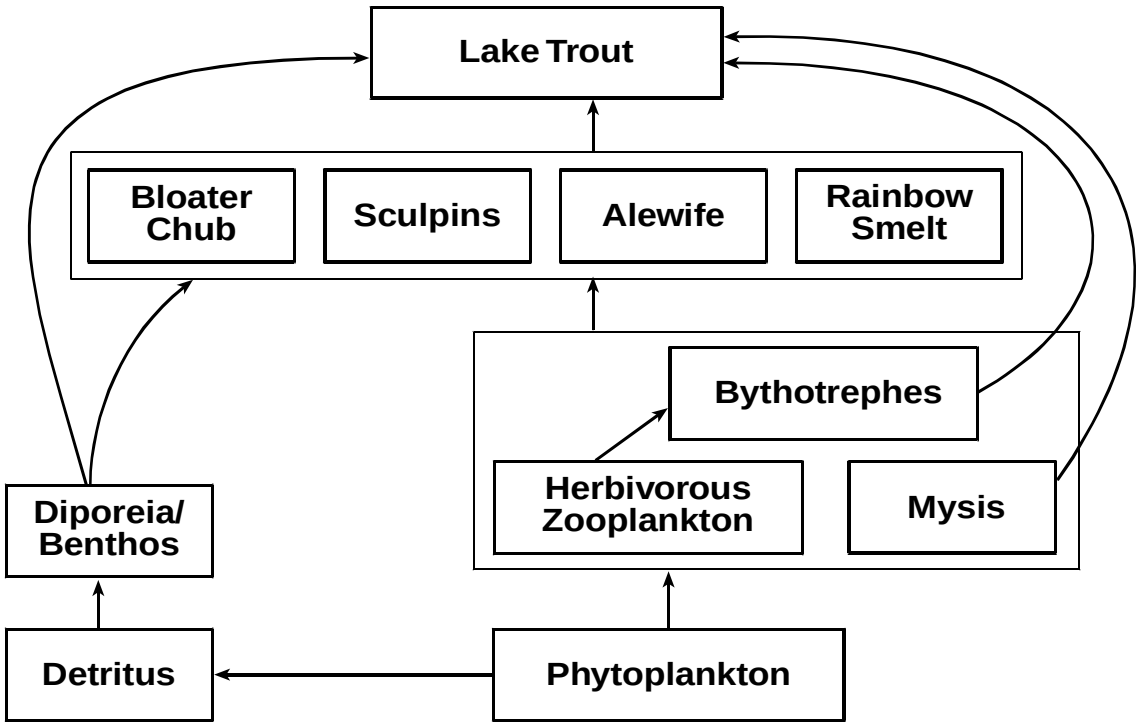


Figure 4. Lake trout food web in Lake Michigan.

species) is beyond present analytical and modeling capabilities. As identified in *Mercury in the Great Lakes: Management and Strategy* (Rossmann *et al*., 1993), the development of such capabilities must initially take place on small, constrained ecosystems as opposed to the Great Lakes. This is consistent with the research approach of Porcella (1992) in developing the Electric Power Research Institute (EPRI) Mercury Cycling Model, which was based upon data gathered from Little Rock Lake and other bog seepage lakes in Wisconsin.

A number of FDCHN enhancements will be considered in the Lake Michigan application. These include incorporating specialized sub-models for phytoplankton (Swackhamer and Skoglund, 1993) and *Diporeia* (Landrum *et al*., 1992), the organisms at the base of the pelagic and benthic food webs. The bioaccumulation process formulations of Gobas (1993), Barber *et al*. (1991), and Sijm *et al*. (1992) will be reviewed for possible updating of FDCHN toxicokinetic descriptions. The detailed bioenergetics model of Hewett and Johnson (1991), which is currently employed in simplified form in FDCHN, may also be more fully incorporated in the model. Finally, a individual-based modeling (IBM) approach may be tested, if individual fish are sampled during the EMP.

Atmospheric Transport and Deposition

Current estimates suggest that atmospheric deposition is the major source of several contaminants to Lake Michigan, including PCBs (Pearson, 1994), and mercury (Rossmann *et al*., 1993). In addition, net volatilization to the atmosphere may be the predominant loss mechanism for semi-volatile contaminants such as PCBs from Lake Michigan (Endicott *et al*., 1992) as well as Lake Superior (Jeremiason *et al*., 1994). Due to the importance of the deposition and exchange of toxics between Lake Michigan and the atmosphere, air-water fluxes of contaminants must be accurately predicted. This will be accomplished initially by observation-based interpolation/extrapolation of atmospheric monitoring data. A longer-term objective

will be to model the deposition and exchange of contaminants by linkage and coupling between the CTF model and a compatible atmospheric transport model. The Regional Particulate Model (RPM) is being developed by the USEPA NERL as the atmospheric model for this application. Based on discussions at an air/water modeling workshop held on 14-15 June 1995 in Detroit, there appears to be sufficient air emissions information for atmospheric simulations of atrazine and mercury only. There does not currently appear to be enough information about air emissions of PCB congeners and TNC to allow a scientifically credible simulation of the atmospheric transport and deposition of these substances.

A. Observation-Based

Observation-based interpolation/extrapolation of atmospheric monitoring data will be used to estimate over-lake wet deposition, dry deposition, and vapor phase contaminant concentration distributions. These estimates will be based upon: (1) routine monitoring at nine land-based sites, (2) ship-board sampling in conjunction with open water monitoring, and (3) three intensive studies focusing on Chicago as an urban source of air toxics.

Measurements from the Integrated Atmospheric Deposition Network (IADN) and EMP will be used to drive the CTF model. An overview of the procedures to be used for deriving atmospheric loadings from monitoring data is provided in the *Atmospheric Monitoring Overview* and *Appendix 3* of the *Mass Balance Project Work Plan*. The Lake Michigan Atmospheric Technical Workgroup will be responsible for calculating atmospheric loadings. This effort must be coordinated with the Modeling Workgroup to ensure compatibility with regard to contaminants of interest, simulation time periods, and spatial scales.

The primary use of observed atmospheric loadings will be to calibrate the CTF model using the best available information to characterize present conditions. Ambient gas phase observations above the water surface will be used in the air/water surface exchange calculations performed by the CTF model.

B. Atmospheric Transport and Deposition Model

An "engineering" version of the RPM adapted for atrazine will simulate transport above the watershed and lake, the gas/particle partitioning and transformations of atrazine in the atmosphere, and the significant deposition and exchange processes with the watershed and lake. This engineering version of the RPM will use the results of previous simulations of the RADM to determine the total particulate mass loadings and particle size distributions which affect the behavior of particulate atrazine. Atmospheric transport and deposition in both the RADM and RPM is driven by a meteorological model, the Penn State/NCAR Mesoscale Model - Generation 5 (MM5). The MM5 generates diagnostic simulations of wind, temperature, humidity, cloud cover and other meteorological variables using a four-dimensional data assimilation (FDDA) technique to continually correct certain model variables toward observed values during the simulation to control errors. Emission inventory data are used to define contaminant source inputs, although specified boundary condition data may be used to augment emission inventories.

Atrazine will be considered a minor constituent of the total mass loading in the particulate matter and its transport and deposition will be estimated based on the RPM results for sulfate and nitrate particulate matter. Simulations of mercury transport and deposition to Lake Michigan may eventually be obtained from the RPM. However, at this time there is significant uncertainty about the importance of particulate mercury in atmospheric loading and deposition. Since there are already sufficient measurements available to make a credible estimate of the air component of mercury loading to Lake Michigan, the initial focus of this air modeling effort will be on atrazine.

The volatile flux of atrazine may be a significant mass balance component for both the lake and regional atmosphere. Because volatile flux is driven by the temperature and concentration (fugacity) gradients between water and air, contaminant transport and fate models for lake and atmosphere must each use consistent models of the air/water interface to estimate this volatile flux. The RPM, RADM and MM5 all

currently use the same terrain-following vertical model structure with a bottom layer thickness of approximately 80 meters. This definition for the bottom layer of these three air models may require modification to assure consistency with the CTF model.

The diagnostic and analytic capabilities provided through atmospheric modeling can complement observation based loading calculations by providing enhanced temporal and spatial resolution of deposition during time periods consistent with observations. Although this potential for enhancing resolution of the observed input field is important, atmospheric modeling provides an objective method of linking atmospheric sources directly to watershed/water body impacts. Consequently, the atmospheric model should be a valuable tool in the regulatory decision-making process for assessing the aquatic impacts due to modifying emission releases in future or past scenarios. The role of atmospheric modeling and plans for model deployment are discussed further in the Atmospheric Modeling Plan below.

C. Air/Water Linkage

Based on discussion at the air/water modeling workshop in Detroit (June 1995), it was determined that complete computational coupling of the air and water models would not be feasible, at least in the near term, due to the differences in time scales for the important physical processes in the air and water media. The redistribution and reaction of contaminants in the water media occur on time scale that are much longer than those for the air media. Water quality models are typically used to simulate multi-year periods, whereas regional-scale air quality models like the RPM and RADM are rarely applied for periods of longer than a few days due to the amount of computing required. Particulate fluxes of contaminants from the air to the lake are not affected by concentrations in the lake, and downward volatile fluxes can be adequately estimated using observed and modeled water concentration data. Therefore, the RPM will be used to simulate important depositional periods spanning a few weeks or months, and climatology and statistical methods will be used to estimate atmospheric inputs to the Lake Michigan mass balance on time scales of seasons to years.

The linkage outputs are wet and dry deposition contaminant fluxes and near surface atmospheric concentrations. The output fluxes and concentrations will be used to define input atmospheric loads and the gradient for gas exchange for the CTF model. Linkage can also occur in the other direction, where volatilization is treated as a source of contaminants to the RPM. However, this reversed flux from water to air does not appear to be significant for atrazine due to its water solubility. In the future, if the simulation of atmospheric PCB transport and deposition is attempted, a coupling may be necessary between the RPM and the CTF models where the models run simultaneously to simulate the bi-directional transfer and feedback of contaminant mass balances for air and water. In this case, volatile exchange (volatilization or absorption) would be computed based on simultaneous conditions in both the atmosphere and water column.

Watershed Delivery

Transport and fate frameworks may be applied to predict the multimedia delivery of toxics from the watershed to the lake. While contaminant loadings from major tributaries are being monitored as part of the LMMBP, these data alone may not be sufficient to accurately define contaminant inputs from the watersheds, tributaries, and harbors that adjoin the lake. Furthermore, quantifying tributary loads based upon monitoring at the river mouth does not identify sources of toxic chemicals. For instance, atmospheric deposition to the watershed will indirectly contribute to tributary loading. Depending upon the actual source, toxics loading from the watershed may or may not decline over time without action, respond to meteorology, hydrology, or land use change. Modeling these significant loads would produce more complete and accurate load estimates and allow more realistic long-term forecasting ability.

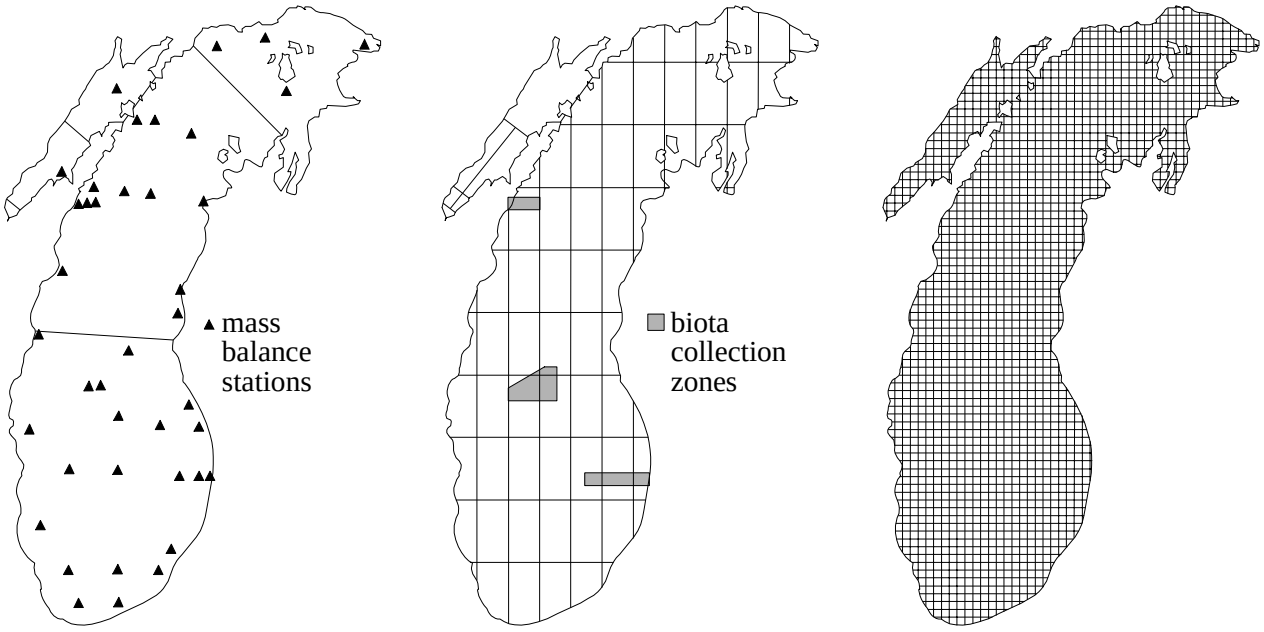
While such modeling capability is important for forecasting purposes, this development should be addressed separately due to the difficulty of managing such efforts within a project of this scope and duration. Development of watershed delivery models is distinct from the lake mass balance model development, because these models simulate toxics transport and fate at fundamentally different scales and have unique data requirements. Furthermore, it is not clear that watershed simulation, on this scale is feasible, at this time. Results

of the LMMBP will be useful for identifying specific toxics and watersheds to prioritize for watershed delivery modeling, based upon the magnitude of tributary loading estimates.

Model Resolution

Model resolution is the spatial and temporal scale of predictions, as well as the definitions of model state variables. While factors such as data availability, model sophistication, and computer resources constrain resolution to a degree, different levels of model resolution are possible and, are in fact, necessary. Three "levels" of spatial resolution, indicated by the segmentation grid of the lake surface, are illustrated in Figure 5. Level 1 is resolved at the scale of lake basins (characteristic length, L = 150 km), with an associated seasonal temporal resolution. This is a screening-level model resolution used in MICHTOX. Level 2 is resolved at a regional scale defined by food webs (L = 40 km) including gross resolution of the nearshore and offshore regions; temporal resolution is weekly-to-monthly. This resolution is roughly comparable to that achieved by models developed in the GBMBS. Level 3 is a hydrodynamic scale resolution (L = 5 km), with associated daily temporal resolution. Level 3 is scaled to resolve and predict particle transport processes as well as hydrodynamic transport.

Although LaMP and Great Lakes Waters Program objectives are “lake-wide”, these emphasize biotic impairments occurring primarily in localized, nearshore regions. LaMP objectives also require that the transport of contaminants from tributaries and other near-shore sources to the open lake be resolved. Therefore, the Level 1 model is not adequate for the study objectives. Level 2 resolution is adequate for most modeling objectives, but not for resolution of significant hydrodynamic and sediment



LEVEL 1
(7 surface water segments)

LEVEL 2
(20 X 40 km surface water grid)

LEVEL 3
(5 km surface water grid)

note: surface sediment segmentation is similar but not identical to surface water segmentation. Biotic zones in bioaccumulation model are superimposed on mass balance model segments.

Figure 5. Surface water segmentation for alternative Lake Michigan mass balance model levels.

transport events. Level 3 resolution is required for accurate hydrodynamic and sediment transport modeling and is desirable for predicting nearshore gradients, especially those formed by transients such as thermal bars, upwelling, and storm-induced resuspension, as well as more persistent features such as tributary plumes, thermal stratification, and the benthic nepheloid layer. Level 3 transport resolution would also be valuable in relating toxics loading from the 10 Areas of Concern (AOCs) adjoining Lake Michigan, which must be addressed by the RAP process, to the LaMP via the LMMBP.

The modeling design for the LMMBP will be based upon the development of several submodels, at two levels of resolution. The CTF model will be resolved at a level comparable to Level 2; the eutrophication model will be resolved at the same level. Because the CTF will be linked to atmospheric fate and transport model predictions, the two will share the Level 2 resolution at the Lake Michigan surface. The POM and SEDZL models will be Level 3 resolution. Results of these transport models will be spatially and temporally averaged prior to coupling to the CTF model. The rationale for specifying different resolutions is that hydrodynamic and predictive sediment transport models demand a Level 3 resolution, and these models offer the best capability for transport simulation and forecasting. A lower resolution is specified for CTF and ESD because these models have been demonstrated at this resolution, and the need for Level 3 toxics resolution is not clear.

Model Quality Assurance

QAPPs will be prepared and implemented for each sub-modeling effort, consistent with MED-Duluth *Quality Assurance Guidelines for Modeling Development and Application Projects*. The QAPPs will specify procedures for code development, testing, modification, and documentation, as well as methods and measures to be applied in model calibration, confirmation, and uncertainty analysis.

Validation

Validation of submodels will include testing for local and global conservation of mass (and continuity), momentum, and energy. Numerical solutions will be tested for properties including stability, convergence, and numerical dispersion, against analytical solutions and output of demonstrated models. These tests will be repeated following model code modifications. Input data, including forcing functions and initial conditions, will be checked by graphical inspection. Averaging and filtering methods used to link models of different resolution, will be tested by repeating tracer simulations in each model and comparing consistently-averaged results.

Calibration

Each of the lake process submodels will require some degree of parameter calibration. However, the overall modeling design is intended to minimize the reliance upon calibration, to better constrain the results. By simulating hydrodynamics and sediment transport, it will not be necessary to calibrate transport in the ESD and CTF models. The toxics transport and fate model will incorporate physicochemical process-based descriptions of partitioning, volatilization, diffusive sediment exchange, and transformation, in order to reduce degrees of parameter freedom. Likewise, the bioaccumulation model will base contaminant uptake and excretion parameters upon process descriptions that separate chemical-specific (K_{ow}) and organism-specific (lipid content) factors. The objective of model design is to construct a framework capable of simulating a wide range of contaminants in a simple, consistent, scientifically defensible manner.

Within each submodel, calibration parameters will be identified. Best estimates for initial values and allowable ranges will be based upon the literature and proceeding model applications. Logs of parameter values tested during calibration will be maintained as documentation of this procedure, along with the appropriate residual statistics. Spatial or temporal variation of parameter values will be allowed only if justified by consideration of the process(es) involved. Although the objective of calibration is to identify optimum parameter values which minimize residual errors, it is necessary to balance the goodness-of-fit with other criteria: for example, the realistic range of the parameters, independent measurements or estimates (and the degree to which these estimates are judged to be reliable), as well as the importance and sensitivity of the various parameters in the model.

Confirmation

Short-term, annual, and long-term model results will be confirmed, to assure that the models and submodels will yield reliable and informative predictions (Chapra and Reckhow, 1983). Confirmation will include model performance evaluation: inspection and quantification of residual errors for state variables, on both local and regional bases. Data uncertainty will be quantified by ANOVA methods. Independent observations, including sediment trap fluxes, water intake, total suspended solids monitoring, vertical current meter and transmissometer arrays, contaminant partitioning distribution data, and predator-prey contaminant ratios, will be used to confirm process submodels. Long-term confirmation will be provided by the radionuclide simulations, and to a lesser extent by performing hindcasts for PCB and mercury.

Goals for Accuracy

The stated goal for model accuracy is prediction of lakewide average concentrations of toxics in water (volume-weighted average), surficial sediment (spatial average), and top predator fish (average fish in each biota zone) within a factor of two of the average concentrations based upon monitoring data. To achieve this model accuracy, loadings and contaminant mass in each compartment must be determined to within 25% of the actual lakewide, annual average value. Approximately 20% of the samples for toxics analyses should be replicates, as a basis for estimating measurement variability. (In this context, replication refers to multiple observations per model segment and sampling interval.) In addition, 75% of loading and ambient samples in all compartments must be quantified for each contaminant (completeness). These data quality objectives are based upon expert opinion, and experience gained in the GBMBS. Failure of the EMP to achieve these goals will degrade the accuracy of the mass balance and model predictions.

Analysis of Uncertainty

It should be recognized that model accuracy refers to a comparison of model predictions to data collected during the EMP. In a forecasting application, the accuracy of model predictions will degrade over time. In either case, parameterization error is a significant source of model prediction uncertainty. To evaluate and quantify the effects of parameterization error, uncertainty analysis will be performed for selected model simulations. The parameter variance-covariance estimation procedure of Di Toro and Parkerton (1993) will be applied to estimate data, parameter, and model error components. With these estimates, confidence intervals for model predictions will be generated using Monte Carlo/Latin Hypercube simulation. Uncertainty analysis will also provide a check on the quality of model parameterization and calibration, via the estimation of parameter errors, which will be applied periodically during model development.

Model Application and Computational Aspects

Annual Simulations

Annual simulations will be run with the integrated submodels for the EMP period of 1994-1995. Results will be analyzed in terms of regional and lake-wide contaminant loads, fluxes and inventories, and spatial and temporal gradients of contaminant concentrations. Bioaccumulation simulations will be analyzed in terms of relative accumulation pathways, spatial and temporal variability of contaminant concentration ratios (BCF, BAF, BSAF, predator/prey), and influence of diet, age, and migration factors. As indicated above, annual simulations for hydrodynamics and sediment transport will also be developed for the period 1982-1983. This will provide four years of transport data, which will be "sampled" to construct synthetic transport fields for long-term CTF simulations. Deviation of climatic, meteorological and limnological conditions during the EMP, from expected conditions based upon the long-term record will be investigated.

Long Term Simulations

Long term simulations will include both hindcast and forecast applications. CTF forecasts will be performed to determine time to steady state, for both continuing and discontinued loads. Forecasts will also be run to evaluate reductions in exposure concentrations resulting from elimination of tributary and/or atmospheric loading. These forecasts will be propagated through the food web bioaccumulation model for PCBs and TNC, to estimate time for sport fish contaminant concentrations to decline below criteria limits. As described above, SIMPLE model scenarios will be used to test the sensitivity of long-term bioaccumulation predictions to food web dynamics. Based

upon the results of long term simulations, graphs will be developed to illustrate the fundamental loading-concentration relationships, for both transient and steady state conditions.

Computational Requirements

The POM is implemented on Lake Michigan using a 5 km horizontal grid. At this resolution, the Lake Michigan model requires approximately one CPU min/day simulated, or six CPU hours for an annual simulation (based on Cray Y-MP performance). The SEDZL three-dimensional Lake Michigan model will require about 50 CPU hours for an annual simulation. Eutrophication, CTF, and bioaccumulation model CPU requirements are comparatively negligible. Short-term runs will be conducted on high-performance workstations (DEC 2100, 3600, and 4700 AXP), although annual simulations and storage of transport fields (0.5 GB per annual simulation) are only feasible on a supercomputer. The NESC supercomputer will be used for coupling the hydrodynamic model with the sediment and contaminant transport model. Approximately 500-2000 CPU hours (Cray Y-MP) will be required annually to support model development and application.

CPU requirements for the MM4 meteorological model, run using an 80 km grid size and a nested 18 km grid over the Great Lakes would require approximately 1000 Cray Y-MP CPU hours for a one year simulation, and would generate 100 GB of output data.

Model results will be visualized using Advanced Visualization Systems (AVS) software running on the NESC supercomputer, AXP and Sun Sparc workstations. Volumetric modeling of lake model predictions will be used both to assist model development (performance evaluation and comparison to data) and for presentation of results. Simulation of events of specific interest may be animated in AVS, with technical support from NESC and RTP visualization labs.

Modeling Data Requirements

This section defines field data requirements for the Lake Michigan mass balance modeling effort, in terms of how data will be used for model development, confirmation and application. Substantially greater detail of the EMP design may be found in the LMMBP Work Plan. Through work group involvement, the modeling committee has offered input to the EMP design to maximize the utility of the sampling and analytic effort, within the overall project constraints defined by GLNPO. It should also be noted that data management and database development are the responsibility of GLNPO.

Data may be categorized in three groups, according to their usage in the modeling process:

Loadings, boundary and initial conditions, and forcing functions - Data that is specified externally (based upon observations or other models), and input to the model. Loadings are external sources of mass for constituent state variable, including contaminants, sediments, sorbents, and nutrients. Boundary conditions are state variable concentrations in media adjacent but external to the model (i.e., the atmosphere and Lake Huron water across the Straits of Mackinaw). Initial conditions are the concentrations of state variables at the beginning of the model simulations. Forcing functions include other data to which the model responds, such as meteorology.

Constituent observations in water, sediment, and biota - Data that are compared to model predictions of state variable concentrations; they may be either observations of the state variables themselves, or of other constituents used as surrogates for state variables. Model performance is principally evaluated in terms of the residuals (differences) between observations and predictions for state variables. Appropriate spatial and temporal allocation of the point observations is necessary for comparability with model predictions, which are spatially and temporally continuous.

Process data - Data that are used to confirm particular aspects of the model formulation and parameterization. Process data are usually specific in terms of constituents and media, and are based upon field and/or laboratory experiments. Process data is particularly useful in confirming aspects of the model parameterization which is unconstrained by other observations.

Loadings, Boundary Conditions, and Forcing Functions

Loadings and boundary conditions necessary for the toxics, solids, and nutrient mass balances will be based upon monitoring data for the atmosphere, tributaries, and Lake Huron. Continuous estimates of loads, for the 1994-1995 EMP period, will be required for the parameters listed in Table 1. Atmospheric loads from dry and wet deposition will be resolved as weekly averages on the Level 2 model grid. Tributary loads will be computed as daily (for events) or weekly (non-event) averages, for each river. The computation of load estimates is considered the responsibility of Atmospheric and Tributary Workgroups. Boundary conditions of concern to the mass balance include vapor-phase air concentrations, and concentrations of state variables in Lake Huron water. Over-water air concentrations will be estimated, based upon the routine (shore-based) and Air Intensive monitoring data. Water quality data from Station 54M, located in northern Lake Huron, will be used to describe the lake boundary condition.

Meteorological data including wind speed and direction, temperature, and solar radiation will be collected from land and ship-based atmospheric monitoring, NWS surface observing stations, and NOAA mid-lake weather buoys. These data will be used to synthesize over-water momentum and heat flux fields, forcing functions for the hydrodynamic model. Ice cover data will also be used as a model forcing function.

Water Column

Water column monitoring will be conducted to determine the spatial distribution and inventory of mass balance state variables in the lake, on a seasonal sampling basis. State variables to be measured in the water column are listed in Table 2. The basic monitoring program consists of sampling on eight cruises conducted aboard the Lake Guardian. Five cruises (April, August, and October 1994; April and September 1995) will sample the 41 EMP stations; three other cruises (June 1994; January and August 1995) will sample a station subset. On all cruises, enhanced vertical sampling resolution will be obtained at nine open-water master stations. In addition to discrete samples for the parameters in Table 2, continuous vertical profiles of conductivity, temperature and transmissivity will be recorded at all stations. Supplemental water column monitoring data will be provided by NOAA-GLERL (weekly-monthly sampling at several southern basin stations), air intensive studies, biota sampling, and municipal water intake components. The parameters of interest from these data sources are identified in Table 3. PCB concentrations (in all media) are to be reported using a standard congener list according to GLNPO Data Reporting Standards. Surrogate recovery data as well as below-detection limit and below-quantification limit results are required for modeling data reduction. Mercury data will be reported for total mercury and methylmercury (if available).

Sediment

Sediment sampling will be conducted to estimate the distribution of sediments, contaminants, nutrients, and selected other parameters in surficial sediments throughout the lake, as well as the fine-scale vertical distribution of contaminants in selected sediment cores.

The primary use of this data is to define initial conditions, as the sediments contain the largest inventory of contaminants in the system. More than 100 box cores, gravity cores and PONAR grab samples will be collected, providing nearly uniform coverage of Lake Michigan sediment locations and types. Parameters of interest in sediment samples are listed in Table 4. The top centimeter of cores will be sampled as the surficial sediment, as will surface grab samples. Approximately 30 sediment cores from deposition basins will be sampled at 1-cm intervals and analyzed for lead-210, cesium-137, and ancillary sediment parameters; 10 of these cores will also be analyzed for contaminants. Trap material from four near-bottom sediment traps will also be analyzed for parameters in Table 4, to better define constituent concentrations for resuspendable, sediments in non-depositional zones. This data will be augment prior to sediment surveys conducted by Cahill (1981), Robbins and Edgington (1975), and Eisenreich *et al*. (1991).

Biota

Biota will be sampled in defined food webs and zones, on a seasonal basis. The top predators of interest, lake trout and coho salmon, will be sampled as discrete age classes. Based upon the collection success in a particular season and zone, individual as well as composite fish may be analyzed for the parameters in Table 5.

Table 1. Parameters Required for Atmospheric and Tributary Loads

Parameter	Atmosphere	Tributary
PCB congeners, TNC, atrazine (+DEA and DIA), mercury (+methyl if available)	Vapor concentration, wet and dry deposition fluxes	Tributary load
Total suspended solids	Particle size and deposition velocity, wet and dry deposition fluxes	Tributary load
Particulate organic carbon	Wet and dry deposition fluxes	Tributary load
Dissolved organic carbon		Tributary load
Total phosphorus	Wet and dry deposition fluxes	Tributary load
Soluble reactive P	Wet and dry deposition fluxes	Tributary load
Total dissolved P	Wet and dry deposition fluxes	Tributary load
Nitrate-nitrite	Wet and dry deposition fluxes	Tributary load
Total Kjeldahl N	Wet and dry deposition fluxes	Tributary load
Ammonia		Tributary load
Dissolved silica	Wet and dry deposition fluxes	Tributary load
Biogenic silica		Tributary load
Chlorophyll *a*		Tributary load
Chloride		Tributary load
Hardness		Tributary load
Conductivity		Tributary load
Alkalinity		Tributary load
Other data	Rainfall, snowfall, pH, T, relative humidity, solar radiation, wind speed ad direction, wave height	Flow, velocity, stage, T, transmissivity, pH, D.O.

Table 2. Water Column State Variables

Parameter	Phases/Comment
PCB congeners	Dissolved and particulate
TNC	Dissolved and particulate
Atrazine (+ DEA and DIA)	Dissolved and particulate (master and biota stations)
Mercury (+ methyl)	Dissolved and particulate (master and biota stations)
Total suspended solids	
Particulate organic carbon	
Dissolved organic carbon	
Total phosphorus	Total and dissolved
Soluble reactive P	Dissolved
Nitrate-nitrite	Dissolved
Total Kjeldahl N	Total
Ammonia	Dissolved
Dissolved silica	Dissolved
Biogenic silica	Particulate
Chlorophyll *a*	
Chloride	
Hardness	
Alkalinity	
pH	
Secchi disk	
Light extinction	
C-14 primary production	Master stations
Phytoplankton (abundance and biovolume)	Master stations

Table 3. Supplemental Water Column Monitoring Data

Study Component	Parameter
NOAA-GLERL Monitoring	Total phosphorus
	Soluble reactive phosphorus
	Nitrate, ammonia
	Dissolved and particulate silica
	Chlorophyll *a*
	Particulate organic carbon
	Dissolved organic carbon
	Chloride
	Temperature
	Secchi disk
	Bacteria, phyto- and zooplankton counts
Air intensive	Wind and wave height
	Volatile flux (PCB congeners, mercury)
	Over-water deposition fluxes (PCB congener, TNC)
	atrazine, and mercury
Plankton sampling (phyto-, zooplankton, and detritus) particle fractions)	Dry weight/volume
	PCB congeners, TNC
	Mercury
Remote sensing (NOAA)	Surface temperature and reflectance
Municipal water intake	Temperature and transmissivity (calibrated to TSS)

Table 4. Sediment Parameters of Interest

Parameter	Surficial Sediment	Sediment Cores	Sediment Traps
PCB congeners	All	Selected	Composite
TNC	All	Selected	Composite
Atrazine*	Selected		
Mercury	All	Selected	Composite
Total organic carbon	All	Selected	All
Cumulative dry weight		Selected	
Gross particle downflux			All
% moisture	All	All	
Porosity (derived)	All	All	
Grain size	All	All	All
Pb-210 and Cs-137	All		All
Total phosphorus	All		All
Extractable/bioavailable	All		All
Total nitrogen	All		All
Ammonia	All		
Total Kjeldahl N	All		
Biogenic silica	All		All

*Selected sediment samples should be analyzed for the presence of atrazine, even though this contaminant is not believed to associate with sediments.

Table 5. Biota Parameters

Parameter	Top Predators	Forage Fish	Invertebrates	Phyto-, zooplankton, and detritus fractions
Age	X			
Weight	X	X	X	
Length	X	X		
Sex	X			
% Moisture	X	X	X	X
% Lipid	X	X	X	X
POC				X
PCB congeners	X	X	X	X
TNC	X	X	X	X
Mercury	X			X
Atrazine				X (+ methyl, if available)

Individual-based sampling provides better information as to the source of contaminant variability. Forage fish will be collected in conjunction with top predators, and analyzed as composites according to size. Invertebrates (*Mysis* and *Diporeia*) will also be sampled at the same times and locations as fish; phytoplankton and zooplankton will be sampled in conjunction with water sampling cruises.

Transport

Additional data will be required to confirm transport simulations. Remote sensing of lake surface temperature and reflectance (a surrogate for suspended solids at the lake surface), municipal water intake measurements of temperature and transmissivity (correlated to suspended solids), and vertical instruments arrays measuring temperature, transparency, depth and current velocity will temperature and transmissivity (correlated to suspended solids), and vertical instruments arrays measuring temperature, transparency, depth and current velocity will provide information about water and particle transport transients at a resolution not attainable by conventional ship-based sampling. Wave height data from ship and buoy observations will be used to confirm the wave submodel used in the transport simulations.

Particle and Contaminant Fluxes

To obtain accurate mass balance results, large-magnitude contaminant and particle fluxes between the atmosphere and the lake, and the lake and the sediment, will be monitored. These include atmospheric wet and dry deposition, net volatilization flux, and net settling and resuspension rates. Monitoring for wet and dry deposition fluxes will be conducted during routine and intensive atmospheric sampling; volatilization flux at the lake surface will also be monitored during intensive ship-based sampling. Sequencing sediment trap arrays will be deployed at deep water locations, to measure settling and resuspension fluxes for solids, POC and selected nutrients (Table 4). Sedimentation fluxes will be determined from Pb-210 profiles in sediment core samples, sediment mixing depth from Cs-137 profiles, and sediment focusing factors from Pb-210 and Cs-137 inventories.

Contaminant Partitioning

All water column contaminant samples will be separated into dissolved and particulate fractions by filtration, and will be accompanied by measurements of total suspended solids, POC, and DOC. Although this data will provide the basis for confirming the description of partitioning in the CTF model, additional data will be required to define the contaminant distribution between sorbent phases within these fractions. These include the organic carbon partition coefficient, K_{oc}, the DOC partition coefficient,

K_{doc}, and the biotic and detrital fractions of POC. The partition coefficients will be treated as contaminant-specific parameters, and will be based upon the literature as well as process data from laboratory experiments. POC fractions will be based upon surrogate measures, including chlorophyll, developed from phytoplankton sampling and biovolume data. Contaminant partitioning in sediment pore water will be described using data from the literature and from field and laboratory experiments.

Contaminant Transformation

Transformation between state variables is of concern for atrazine, mercury, and PCB mass balances. Because atrazine is known to degrade in soil as well as water, the concentration of diethylatrazine and deisopropylatrazine will be measured with the parent compound in all tributary and water samples. These data will confirm the location and rates of atrazine transformation. Mercury methylation and demethylation rates are not being measured for the LMMBP, consistent with the total mercury mass balance objective. Operationally, a sediment equilibrium constant between organic and inorganic mercury states will be defined for CTF modeling, based upon the literature. PCB congener dehalogenation rates will be estimated from data in the literature. Prior modeling efforts, including the PCB mass balance models for Green Bay and the Fox River, as well as process research (Rhee *et al.*, 1993) have suggested that dehalogenation is probably negligible for the range of PCB sediment concentrations observed in Lake Michigan.

Resuspension

The relationship between shear stress and resuspension rate is critical for sediment transport modeling, and must be measured for representative sediments throughout the lake. Although a number of flume devices have been used in the laboratory for this purpose, the bottom-resting seaflume (Hawley, 1991) has been deployed previously in the Great Lakes. For this project, the seaflume will be modified to improve quantitative results, and deployed to test sediment resuspension properties at master stations, sediment trap and vertical instrument array locations, and other locations to obtain data for a variety of sediment substrates. This information will be used to estimate resuspension properties throughout the lake, based upon the spatial distribution of sediment physical properties.

Eutrophication

Specialized process measurements required for the eutrophication model include C-14 primary production, phytoplankton and zooplankton abundance and biovolume, light extinction, and incident solar radiation.

Bioconcentration and Bioaccumulation

Species- and contaminant-specific toxicokinetic parameters required for the bioaccumulation model, will be based upon the literature and prior modeling studies. This parameterization will be refined by calibration to biota contaminant data.

Data for movement and migration patterns, feeding habits, and seasonal growth rates of fish are also required for the bioaccumulation model. Fish are not perfect integrators of lake-wide toxics exposure; rather, their contaminant burden reflects their exposure (particularly through diet) along a chemical gradient defined by their movements over seasons and years. National Biological Survey (NBS) personnel interviews, reports and file data will be used to construct fish migration patterns. Feeding habits will be based upon gut contents analysis for top predator and forage fish. Age-weight relationships will be developed for the collected fish, to define their rate of growth at each collection location.

Supporting Studies List

A draft LMMBP work plan was distributed for public comment by GLNPO in October, 1993. A substantial number of comments were received, including suggestions for research and additional monitoring to support the mass balance objectives. These suggestions were organized, and the following list of candidate "supporting studies" was developed:

Candidate Supporting Studies for LMMBP:

- Measure contaminant concentrations in plankton; confirm separation of phytoplankton, zooplankton, detritus.

- Monitor movement/migration of food web fish species.

- Gut contents analysis (diet composition by weight; gut fullness) to define food web structure and seasonal variance.

- Measure rates of contaminant uptake by phytoplankton, including relationship between uptake and growth.

- Measure seasonal changes to invertebrate growth and lipid.

- Routes of contaminant transfer to benthic organisms; linkages between food web structure and contaminant concentrations in invertebrates; dietary composition and feeding behavior of *Diporeia* and *Mysis*.

- Measure rates of uptake (diet/dermal/respiration) and elimination (respiration/excretion/ metabolism) for PCB congeners and TNC in lake trout, alewife, and smelt.

- Study role of lipid transfer and synthesis upon hydrophobic contaminant accumulation by invertebrates.

- Research of sediment bioturbations by sculpins, *Mysis, Diporeia*, etc.

- Improve biotic carrier (birds, insects, fish) flux estimates for contaminants.

- Measure transformation rates of atrazine in Lake Michigan.

- Measure air-water exchange fluxes for contaminants.

- Determine effect of chemical hydrophobicity/ lipophilicity (K_{ow}) and XAD-2 resin separation efficiency for dissolved and DOC-bound phases.

- Research the effects of sampling equipment upon dissolved HOC measurements and blanks.

- Study fate and bioavailability of atmospheric particulate matter in the water column.

- Measure methyl mercury in water, sediment, and biota for understanding mercury cycling and bioaccumulation.

- Analyze PCDD, PCDF and coplanar PCB congeners in sediment and fish.

- Process research on mercury species transformation, sorption, and bioaccumulation.

- Measure sediment nutrient fluxes.

- Study organic carbon sorbent kinetics (especially particle degradation/mineralization rates): vertical resolution in water column/BNL/sediments.

- Improve measurements or estimates of flow across Straits of Mackinaw.

- Acquire/interpret remote sensing data for surface temperature, total suspended solids and chlorophyll.

- Water intake monitoring for temperature and transmissivity.

- LMMBP integration with University of Michigan/NOAA thermal fronts study.

- Measure tributary contaminant loading during high-flow events.

- Estimate solids load from shoreline and bluff erosion.

- Monitor other significant point source loads for evaluating effectiveness of load reduction efforts.

- Research and estimation of contaminant loading from storm sewers/urban runoff.

- Model coupling of atmospheric and lake mass balances for hazardous air pollutants.

- Watershed deliver modeling to estimate present and future tributary loading of nutrients, solids and contaminants.

- Develop methods of distinguishing and separating particles into biotic and abiotic, as well as functional organic carbon sorbent classes.

- Fine-scale mapping of density, porosity, particle size and organic carbon content of surficial sediments based upon acoustical profiling or sediment surveys.

- Measure sediment mixed layer depth, particle residence time, and sedimentation velocity throughout depositional zones by coring and Cs and Pb-210 radiodating.

- Measure particle and contaminant exchange between sediment and water column: sediment trap measurement of vertical fluxes of solids, POC, Cs and Be, chlorophyll, nutrients, and selected contaminants.

- Measure sediment resuspension properties as function of shear stress.

- Measure rates of contaminant desorption from resuspended sediment particles.

- Sampling and analysis of sediment pore water chemistry.

- Measure in-lake temperature, current and suspended solids profiles.

- Measure particle settling velocity (including effects of flocculation).

- Research and measurement of dissolved and DOC-bound contaminant exchange between sediment and water.

The final selection of supporting studies necessary to support the modeling effort for the LMMBP, was based upon prioritization of modeling data requirements, utility in relationship to the model paradigms, and availability of demonstrated methods. Several supporting studies have been funded, as described in Extramural Plan below. However, at this time a number of high-priority efforts have not been initiated, due to lack of adequate time for planning, funding and personnel shortfalls, and constraints upon extramural modeling vehicles. These efforts are described below:

Eutrophication/Sorbent Dynamics (Research and Submodel)

The ESD model will require development or modification of existing models, to refine the relationships between biotic and organic carbon state variables, and to incorporate linkages to hydrodynamic and sediment transport submodels. In addition, research of specific processes related to understanding and modeling the dynamics and transformations of organic carbon states in Lake Michigan will be important to develop and accurate, scientifically-defensible toxics mass balance model. In Lake Michigan, the loss and transformation of particulate organic carbon states appears to be particularly significant (Eadie *et al*., 1983; Eadie, 1987). Accurate simulation of the sorbent dynamics is critical, because the major transport, fate and bioaccumulation processes for toxics are all mediated by partitioning.

Sediment Transport Process Measurements

Measurement of sediment resuspension properties is essential for accurate sediment transport simulation. The measurements should establish the relationship between resuspension rate and applied shear stress, for an appropriate range of shear stresses both above and below the critical shear stress, including consideration of the effects of sediment ageing, compaction, and armoring. Methods for extrapolation of results to the whole lake, such as acoustical impedance, should be tested in conjunction with sediment coring. This research should evaluate the variation in sediment resuspension properties both vertically and areally (at different spatial scales), as well as the relationship between resuspension properties and sediment contaminant concentrations. Although aspects of this process may be addressed by deployment of the seaflume, continued development will be necessary to ensure compatibility with modeling requirements.

Estimates of Shoreline Erosion Load: Dynamics and Variability

According to both contemporary (Colman and Foster, 1994) and historical sources, bluff and shoreline erosion is the major component of sediment loading to southern

Lake Michigan. Although the majority of the erosional load is sand, as much as 25% is fine-grained material. Both components are probably significant influences upon sediment and contaminant transport. To be useful for modeling, the estimates of coarse- and fine-grained erosional loading must be resolved in terms of both temporal and spatial distribution. Estimates based upon relationships to factors such as wind and wave intensity, and water level, could be incorporated in the sediment and contaminant transport model. Survey of the literature reveals no such estimation methods, however.

Vertical Contaminant Concentration Profiles in Sediment

Analysis of the top 1 cm of sediment cores, was recommended by the Sediment Workgroup as the optimum method to sample the distribution of toxics in the surficial mixed layer of lake sediments. From a mass balance perspective, this data will provide an adequate measure of the resuspendable toxic chemical associated with the sediment. Additional sampling of deeper sediment layers will be necessary to measure sediment-associated toxics at locations in the lake where greater than 1 cm of sediment resuspension is predicted, as well as to define vertical contaminant gradients which will increase contaminant fluxes via sediment mixing, bioturbation, and benthic irrigation processes. Analysis of sediment cores collected in 1991-1992 may satisfy this latter need, at least for PCBs. However, sediments subject to greater than 1 cm of resuspension will be located in shallower lake regions, areas where coring and vertical profile analyses have not been performed. Because sediment core samples will be archived, it may be possible to defer analysis until estimates of maximum resuspendable depth can be obtained from the sediment transport model.

Volatilization Mass Transfer Rate

The volatile exchange of semivolatile toxics is driven by the local concentration gradient between the water and air, at a rate specified by a volatilization mass transfer coefficient (k_v). k_v is generally estimated using semi-empirical relationships based upon two-film, surface renewal, and penetration mass transfer descriptions. Depending upon the relationship chosen, k_v estimates can vary by as much as a factor of 5-10, directly influencing the computation of volatile flux. Furthermore, the different relationships vary in terms of k_v sensitivity to environmental variables including wind speed, wave height, fetch. For semi-volatile contaminants in Lake Michigan, this variability introduces considerable uncertainty into the mass balance. Although measurements of volatile flux have been performed for toxic chemicals in the laboratory, and for tracers (O_2, CO_2, H_2O, Rn) in streams, lakes, and oceans, direct environmental measurements are necessary in Lake Michigan to measure volatile exchange of hazardous air pollutants, especially PCBs and mercury.

Tributary Sampling During Sediment Resuspension/Transport Events

Highly-resolved monitoring and detailed modeling of sediment and contaminant transport in Great Lakes tributaries, has demonstrated that tributary loading is strongly related to extreme high flow events for contaminants originating from tributary sediments (Gailani *et al*., 1994; Velleux and Endicott, 1994). Unless the EMP monitoring program samples such events in tributaries with significant in-place pollutants, it is likely that tributary loading will be significantly underestimated. It is unclear whether the EMP tributary sampling effort can adequately address this requirement, in particular the "first flush" of contaminants which occurs on the rising limb of the hydrograph.

Watershed Contaminant Delivery Model

The need for a watershed component to the LMMBP was described above. Depending upon the specific toxic chemical, watershed delivery encompasses a number of source and transport pathways. For atrazine, the source is spring agricultural application; runoff and groundwater transport from cultivated land are principal transport mechanisms. For PCBs and mercury, some combination of atmospheric deposition, nonpoint sources, and contaminated sediments appear to serve as watershed sources. Unless mass balance analysis is applied on the watershed, as it will for the atmosphere and lake, relationships between sources and tributary loading necessary for load reduction efforts will not be established. The severity of such a limitation upon the utility of the modeling results for each contaminant, will depend upon the magnitude of the watershed load relative to both air/water and sediment/water mass fluxes. Relative magnitudes of contaminant loads and mass fluxes will be determined as part of the mass balance project,

suggesting that a watershed contaminant monitoring and modeling effort be designed and conducted subsequent to this project. Tributary monitoring and load estimates will also serve to identify specific watersheds for contaminant delivery modeling efforts.

Development of User Interface and Model Integration System

The drawback of the linked submodel framework, is that model execution and data transfer become a complex, repetitive series of computer operations. Thus, use of the models is beyond the general capabilities of scientists and decision-makers, thereby limiting interaction with the models for both scientific and managerial interests. This situation would be greatly improved if the processes of model development and application was systematized and automated. To this end, a computer-based model integration system should be developed for the LMMBP models, with graphic user interfaces constructed for data analysis, model visualization, scenario management, etc. Such development would greatly facilitate the accessibility and utility of the models.

In-House Plan (MED-Duluth/LLRS)

The MED-Duluth/LLRS inhouse modeling team will lead the lake mass balance modeling effort. They will be responsible for the following tasks:

Screening-Level (MICHTOX) Analysis

The screening-level mass balance analysis performed for PCBs will be extended to the other toxics of concern: atrazine, mercury, and TNC. This will provide an operational model for evaluating transport and fate pathways for the different contaminants, testing air model linkages, and rapid incorporation of toxics loading and ambient monitoring data into the mass balance. The screening model will continue to serve its present function as a means of communicating and demonstrating the mass balance paradigm.

Submodel Development and Linkage

The inhouse team will lead development of the sediment and contaminant transport, CTF, and food web bioaccumulation models and model linkages.

Green Bay Prototype Application

The integrated submodel framework will be prototyped on Green Bay, using the GBMBS data for testing and confirmation. Sediment and contaminant transport, CTF, and food web bioaccumulation submodels will be linked to simulate the 1989-1990 mass balance for PCBs and lead in the Fox River/Green Bay ecosystem. The extensive data for suspended solids, PCBs, and lead will allow for comprehensive testing of the Lake Michigan submodels, except that Green Bay Organic Carbon Based Sorbent Dynamics Model (GBOCS) (DePinto *et al*., 1993) will be substituted for the ESD model. Such a test application is necessary for productive model development in advance of the EMP data.

Model Development for Lake Michigan

The inhouse team will perform data reduction, construction of input data sets, calibration and confirmation of the sediment and contaminant transport, CTF, and food web bioaccumulation models. Linkages with the eutrophication/sorbent dynamics and atmospheric transport models will be established.

Lake Michigan Model Application

The integrated submodel framework will be applied to Lake Michigan, including both short- and long-term simulations for both scientific and managerial objectives.

Extramural Plan

The expertise of a large number of extramural researchers will be required for a successful LMMBP modeling effort. Academic, consultant, and government collaborators will be funded to provide specialized expertise including: submodel process formulation, experimental design and conduct, data analysis, model development, and scientific peer review. Several cooperative agreements are in progress to develop and parameterize transport, fate and bioaccumulation process descriptions, funded by an MED-Duluth/LLRS initiative for reducing uncertainty in toxic chemical models for the Great Lakes. These include:

Colloid Mediated Transport of Hydrophobic Organic Contaminants Across the Sediment-Water Interface in the Great Lakes Ecosystem (Yu-Ping Chin, Ohio State University) Development and application of

methods to characterize and quantify organic colloidal matter residing in the pore water of Great Lakes sediments, study the effect of pore water colloids upon HOC distribution, and estimate on the basis of experimental measurements the ability of porewater colloids to facilitate the exchange of HOCs between the sediment bed and the overlying water column.

Reducing the Uncertainty in Modeling Dietary Transfer of Hydrophobic Contaminants (Robert Thomann, Manhattan College) Investigation of the dietary accumulation process of HOCs from detrital organic carbon to a benthic invertebrate species, leading to an improved submodel for macrobenthos bioaccumulation.

An interagency agreement between MED-Duluth/LLRS and the NOAA-GLERL has been established to fund the following research:

Accumulation and Mixing of Recent Sediments in Lake Michigan Collection and dating of sediment cores taken at various locations in the lake, to generate lakewide distributions of sedimentation rate, mixed layer thickness, and Cs-137 and excess Pb-210 inventories.

Bioaccumulation of Organic Contaminants by *Diporeia* spp.: Kinetics and Factors Affecting Bioavailability Investigation and modeling of bioaccumulation rates of PCB congeners, including factors such as temperature, sediment composition, and availability of fresh detritus. Rates of porewater irrigation by *Diporeia* will also be measured.

Hydrodynamic Model of Lake Michigan Development and confirmation of a three-dimensional hydrodynamic model, as described above.

Sediment Resuspension and Transport in Lake Michigan Instrument platforms will be deployed to measure vertical water column distributions of temperature, transparency, and current at selected locations in the lake. Seaflume device will be deployed to measure sediment resuspension properties.

Sorption, Flux and Transport of Hydrophobic Organic Chemical (Wilbert Lick, University of California) Study of sorption process for HOCs on fine-grained sediment particles and incorporation of this information into CTF models. Experiments will be performed to measure equilibrium partition coefficients and chemical sorption rates to and from sediments, under well-controlled conditions, in both suspended solids and deposited bottom sediments.

Uptake and Loss of PCBs by Phytoplankton: Importance to Mass Balance Models (Deborah Swackhamer, University of Minnesota) Investigation of the relationship between phytoplankton growth and HOC uptake kinetics, and HOC loss from phytoplankton by desorption and exudation. A submodel describing the dynamics of HOC accumulation in phytoplankton will be developed to incorporate this experimental data.

Use of Sediment Traps for the Measurement of Particle and Associated Contaminant Flux in Lake Michigan Deployment of sequential-sampling sediment traps, to measure gross downward fluxes of particulate matter and organic carbon, and to collect and analyze samples of the resuspendable sediment pool from selected depositional and non-depositional regions of the lake.

Additionally, several aspects of the EMP sediment sampling program (sediment core collection, radiometric dating, analysis for contaminants) have been coordinated with other programmatic missions and funding sources, including the MED-Duluth/LLRS Mercury Fate and Accumulation Project and the ERL-Duluth Great Lakes EMAP Project.

A number of vehicles may be used to address the needs for additional supporting studies identified above. These include solicitation and competitive selection of cooperative agreements, funding work assignments through existing Agency contracts, and interagency agreements.

Schedule

The schedule for LMMBP model development is complicated, for it must accommodate a number of incongruous objectives and factors: substantial model development lead time, uncertainty as to the schedule of data delivery, potential disruption of extramural vehicles,

lack of funding to initiate necessary modeling tasks, and institutional requirements to rapidly develop interim and final results. In particular, timely project completion will be contingent upon stable funding, staffing, and extramural vehicles. Interagency agreement, cooperative agreement, and inhouse model development efforts have already begun, with additional model development efforts initiated in FY95. It is expected that a reasonably complete EMP data set will not be available until 1997, allowing two years for model development and testing, Green Bay prototype application, and conduct of supporting research. Initial simulations from the hydrodynamic and sediment transport models will provide transport linkages to ESD and CTF models in late 1995 and 1996. By 1997, the linked submodels will be operational, although confirmation and refinement of simulations for the EMP period (1994-1995) will require another year. Long-term model simulations will be conducted in 1998. Project completion, including preparation of final reports and transfer of the modeling system to GLNPO, is expected in 1999.

Atmospheric Modeling Plan

Introduction

Atmospheric modeling provides a direct link between air toxics emissions and the greater Lake Michigan watershed. The Atmospheric model should be viewed as a comprehensive system, including not only the air quality simulation model (AQSM) which provides concentration and deposition fields, but also the meteorological and emissions models required to drive the AQSM. The atmospheric modeling system provides the following information useful to the aquatic mass balance model:

1. direct wet and dry deposition loadings,

2. near-water, ambient gas phase concentrations used in mass balance surface exchange calculations,

3. meteorological fields of wind speed and direction, air temperature, heat flux, and radiation to drive hydrodynamic processes influencing sediment/water exchange, air/water exchange, and water column advection and dispersion.

As stated previously, sufficient air emissions data do not currently exist to allow a credible simulation of the transport and deposition of PCBs and TNC. The focus of the atmospheric modeling effort will be on atrazine, with a possible treatment of mercury if project resources allow. The interaction between the air/water interface may be bidirectional for certain toxic substances. During certain time periods, volatization of PCBs from the lake surface will increase ambient air concentrations over water, and may act as a major source in itself for downwind receptors. In order for PCBs to be adequately modeled for the purposes of determining the overall mass balance for Lake Michigan, new and advanced model coupling techniques will likely need to be developed which are not included in this modeling plan. Since the focus of this effort will be on atrazine, and atrazine is not known to be significantly volatilized from the lake surface, a one-way flux from air to water will be modeled. Atmospheric modeling will assist near-term program specific tasks and process oriented research by:

1. providing concentration and deposition fields for aquatic mass balance inputs,

2. supporting regulatory analyses addressing impacts resulting from various emission control strategies,

3. serving as an integrator of available information (e.g., emissions, meteorology, ambient air chemistry) to enhance our understanding of transformation and deposition processes and provide direction for continued research.

The following plan describes the near-term (1995-1996) and long-term approaches for regional scale atmospheric modeling within the Mass Balance Project.

Air Quality Simulation Model

A. Model Description

A dual track model development effort will address near-term program needs and research interests for the LMMBP. Modeling will be based on variations of the RADM and the RPM, which utilize a gridded Eulerian framework to treat the relevant transport, transformation and deposition processes. The dual track reflects an immediate model development objective to be program responsive and the ongoing interest in enhancing the scientific credibility of the modeling efforts toward reducing uncertainty and

improving process level understandings. The operational and research grade models will be based on similar geometric frameworks, thus minimizing the interfacing with meteorological, emissions and aquatic mass balance models. Generally speaking, the operational model will incorporate highly parameterized and available chemical transformation, particle description, and deposition schemes. Research grade modeling will build upon operational-grade models by incorporating improved process characterizations utilizing process-related observed data and more sophisticated, mechanistic treatment.

Spatial scales. The modeling domain will extend throughout the continental U.S. (perhaps extending westward only to the Rocky Mountain region) and consist of a double-nested horizontal grid arrangement of 54 km and 18 km grids (this may change to a 60/20 configuration). The 18 km grid would overlay the Great Lakes basin. Generally 15 vertical layers will be used to represent the atmosphere through 100 mb (roughly 15 km). Some preliminary modeling may be conducted with 80 km grid cells and 6 vertical levels to test newly coded parameterization schemes. Certain research grade models may be based on 25 vertical levels for improved characterization of meteorological processes affecting vertical mixing and transport.

B. Operational Model

The operational model will be based on simplified treatments of particle characterizations, chemical transformations and deposition. Gas phase chemistry of oxidants and relevant radical initiation/destruction processes will be simulated by a preliminary RADM application, rather than calculated explicitly with complex chemical and physical mechanisms for particulate matter in the RPM. For example, particle concentrations and size distributions will be estimated in the RPM from the pollutant concentration data obtained from the RADM simulation. Phase distribution between particles and gas-phase will be based on best available thermodynamic data. Similarly, deposition processes will utilize existing algorithms and available data. Basically, "off-the-shelf", highly parameterized components will be used to economize model development and CPU times, respectively. For discussion purposes, the operational model will be referred to as the "engineering" version of the RPM. A working version of the operational model is now being developed and should be complete in early 1996.

C. Research-Grade Modeling

Using the same general model structure as the operational model, the research-grade model would be enhanced through continual updating of parameterization schemes and the incorporation of mechanistic chemistry and particle characterization algorithms. The research grade model will be referred to simply as the RPM, a derivative of RADM including treatment of sulfur, nitrogen and organic-based aerosols relying on more deterministic treatments of gas and aqueous-phase chemistry and phase distribution processes. Application of the RPM would not require a previous application of the RADM.

Meteorological Modeling

A. Model Description

Meteorological information for the toxics transport and deposition modeling will be obtained from the Penn State/NCAR Mesoscale Modeling System - Generation 4 (MM4) and Generation 5 (MM5). The MM4 and MM5 are Eulerian-grid, primitive-equation meteorological models which can employ four-dimensional data assimilation (FDDA) for diagnostic applications to constrain their simulations to the observed conditions. They can also be used for prognostic applications, but typical model error growth limits these forecast periods to about 48 hours. The MM5 has been developed as an extension of the MM4 to allow non-hydrostatic modeling of atmospheric physics. This Eulerian model, when using the non-hydrostatic physics, can resolve horizontal scales down to 4 km. It has improved computational grid nesting capabilities to allow up to nine simultaneous grids with the capability of moving nests to follow small-scale phenomena of interest (squall lines, mesoscale convective complexes, etc.). Initial applications will use existing model output from the MM4 at an 80 km horizontal grid scale and 15 vertical levels. Meteorological information on a

smaller horizontal scale will be produced using objective spatial analysis schemes and interpolation.

MM5 applications should be possible beginning in late 1995.

Inputs required by the MM4 and MM5 models include: hemispheric-scale meteorological model analyses from the U.S. National Meteorological Center (NMC) and/or from the European Center for Medium-Range Weather Forecasting (ECMWF), terrain height and surface type information at the horizontal scale of the modeling grid, observed meteorological data at the Earth's surface (at three-hour intervals for FDDA applications), and observed meteorological data at various vertical levels in the atmosphere (at 12-hour intervals for FDDA applications). Normal model outputs include: horizontal wind vectors, temperature, water vapor mixing ratio, atmospheric pressure, convective (sub-grid-scale) precipitation and non-convective (resolvable grid-scale) precipitation. Special model outputs obtainable without code modification include cloud water and cloud ice density. Modifications can be made to extract the heat and momentum flux variables that are currently internal to the model code.

The RADM and RPM currently use a meteorological data pre-processor to read MM4 output data and format them for air-quality model input. The MM4 has normally been operated with the same horizontal and vertical grid definition as the air-quality model to which data is provided. Thus, the meteorological data pre-processor is used to simply modify the computational data format. At this point there are no plans to allow feedback of chemical and aerosol results from the air-quality model to the meteorological model. It has been shown that aerosol loading of the atmosphere does affect radiative energy transfers, and these feedback mechanisms could be significant to purely prognostic simulations. However, the MM4 and MM5 will be applied in a diagnostic mode using four-dimensional data assimilation of observed meteorological variables to reduce model errors, and a treatment of radiative energy feedback is not necessary.

We envision that the meteorological model could supply both the air-chemistry model and the hydrodynamic model with meteorological inputs, but both links would be forward only (one-way). We realize that water surface temperature and roughness (wave height) information from the hydrodynamic model could be used to provide feedback forcing to the meteorological model, but such two-way linking would require the same level of effort as two-way linking to the air-chemistry model, which has thus far been beyond the scope of our research and development projects.

B. Meteorological Scenarios

Time periods for modeling will be determined by considering availability of processed MM4 simulations and relevance to the LMMBP. Currently, MM4 has been exercised for 1990 as part of the Interagency Workgroup on Air Quality Modeling (IWAQM) and initial modeling will therefore be restricted to that year. Issues to be resolved include the identification of meteorological periods and the method of producing annual estimates. Limitations on CPU time and storage media may restrict full, 365-day simulations. Consideration will be given to aggregating meteorological episodes to represent reasonable distribution of events in order to reduce total execution time. These computational savings become more important as we progress from operational to research-grade models.

Emissions Data and Modeling

Emissions data at the county level by season are available for mercury and atrazine. These data will be gridded into RADM compatible formats using standard GIS procedures. Eventually, these emission files should be updated as information becomes available from the Regional Air Pollutant Inventory Database System (RAPIDS). The availability of that inventory ultimately will influence the selection (if any) of additional substances to be modeled beyond these two toxics.

Emissions data are not available for restricted/banned chemicals such as PCBs and TNC. The types of modeling analyses for these toxics will be restricted to determining transport patterns from lake surfaces.

Proposed Model Simulations

Atrazine - Atrazine modeling would be performed using the MM5, RADM and the engineering version of RPM for the 1994-1995 study period. One- to two-week simulations would be performed for important depositional episodes and a statistical aggregation technique would be used to estimate concentrations and deposition rates throughout the study period. The RPM would consider particle-gas phase interactions for atrazine.

Mercury - Mercury modeling has been conducted with the RELMAP for the continental U.S. (Bullock, 1997). This modeling effort provided mercury air concentration and deposition estimates on a 40 km horizontal scale. Modification of the RPM to provide higher-resolution mercury concentration and deposition estimates is possible. Transformation and deposition processes would be based on the RELMAP effort with the addition of new gas-phase chemical mechanisms to reflect recent scientific advances.

PCBs and TNC - Modeling is not planned for PCBs or TNC. The LMMBP may want to consider supporting emission inventory work for banned substances such as TNC and PCBs. The value of atmospheric modeling of banned substances for regulatory purposes requires clear definition and understanding before committing large resources.

Interfacing/Linking Issues

A. Unidirectional Linking

The initial modeling efforts will provide unidirectional inputs from the atmosphere to the Lake. The model output will consist of hourly wet and dry deposition and ambient gas phase concentration estimates above the lake surface on an 18 km (or other) basis. An interfacing system needs to be developed to interpolate the atmospheric estimates over comparable lake area domains. Note that the output will include concentration data above the lake surface required for air/water exchange calculations in the mass balance models. An interface should also be developed between the MM4 output files and the hydrodynamic model used in mass balance modeling. Analogous interpolation and extrapolation needs to be performed on monitoring data that are used to provide atmospheric loadings to the aquatic mass balance models. However, the large output files and consistent framework associated with the atmospheric models suggests that a specific, perhaps user friendly, software be developed for this interfacing, particularly if future technology transfer efforts are to be conducted with State agencies.

B. Bidirectional Linking

A longer term objective is the more complete interactive operation of the aquatic and atmospheric models in which the interfacing is imbedded in the modeling construct and the lower atmosphere is impacted by air/water exchange of gaseous species. This linkage is being addressed through USEPA's High Performance Computing (HPCC) program. The end product will be the capability to perform direct source to aquatic effect simulations incorporating more realistic physical treatment of exchange processes, without intermediate interface processing steps.

Atmospheric Modeling Schedule

Time Frame	Products
1/96	Operational engineering version of RPM
4/96	MM5, RADM and RPM modified to fit CTF model grid
1/96-7/96	Engineering RPM adapted for atrazine, results obtained for selected time periods in 1994 and 1995
9/96	Operational RPM with integrated gas and particle mechanisms for sulfates, nitrates, and some organics
9/96-1/97	Long-term atrazine deposition results obtained from engineering RPM using a statistical aggregate technique

Time Frame	Products
1/96-1/97	Construction of model deposition and phase distribution algorithms based on field data and related University cooperative research
	Episodic runs for 1994 intensive period to evaluate full-scale RPM model performance for atrazine
	Refinement of operational engineering RPM
1/97	Begin seasonal aggregation runs with full RPM

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Appendix B
Lake Michigan Mass Balance Project
Modelers' Curriculum Vitae

Contents

Douglas D. Endicott

Environmental Research Engineer
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7613
Fax: (734) 692-7603
endicott.douglas@epamail.epa.gov

Role in the Lake Michigan Mass Balance Project

Responsible for in-house model development and applications.

Education

B.S.E. (cum laude), Environmental Science Engineering, University of Michigan, 1983
M.S.E., Environmental Engineering, University of Michigan, 1984

Professional Experience

Research Environmental Engineer (Modeling Team Leader), USEPA, LLRS, 1988-Present.

Environmental Engineer (Adsorption Treatment Research), Technical Support Division, USEPA, Office of Drinking Water, Cincinnati, Ohio, 1985-1988.

Environmental Engineer (Hazardous Waste RI/FS), Engineering Science, Atlanta, Georgia, 1984-1985.

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Russell G. Kreis, Jr.

Chief, CBSSS
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7615
Fax: (734) 692-7603
rgk@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Liaison between modeling workgroup and biota workgroup. Insure that biological aspects of modeling projects are credible.

Education

B.S., Biology, Eastern Michigan University, Ypsilanti, Michigan, 1972
M.S., Biology, Eastern Michigan University, Ypsilanti, Michigan, 1974
Ph.D., Resource Ecology, University of Michigan, Ann Arbor, Michigan, 1984

Previous Positions

Research Aquatic Biologist, USEPA, LLRS, Grosse Ile, Michigan, 1986-1996

Research Associate, Department of Geology. University of Minnesota, Duluth, Minnesota, 1984-1986

Research Assistant, Great Lakes Research Division, University of Michigan, Ann Arbor, Michigan, 1974-1984

Research Interests and Skills

Great Lakes Ecology and Biology
Algal/Diatom Ecology, Systematics, and Morphology

Professional Societies

International Association for Great Lakes Research (Secretary 1986-1988; Technical Advisory Committee)
Michigan Botanical Society

Other Appointments

Acting Station Chief and Station Group Leader, MED-Duluth, LLRS, Grosse Ile, Michigan, 1995.
Co-Chairman, Green Bay Mass Balance Biota Committee.
Chairman, Green Bay Mass Balance Food Chain Modeling Subcommittee.
Member, ARCS Risk Assessment and Modeling Workgroup (GLNPO).
Member, Great Lakes EMAP Planning Committee.
Member, National Sea Grant Zebra Mussel Review Panel.
Member, Detroit River Remedial Action Sediment Subcommittee.
Member, Detroit River Remedial Action Technical Advisory Committee.
Member, Lake Michigan Mass Balance Biota Workgroup.

Publications

Peer-Reviewed Journals

Velleux, M.L., J.E. Rathbun, R.G. Kreis, Jr., J.L. Martin, M.J. Mac, and M.L. Tuchman. 1993. Investigation of Contaminant Transport from the Saginaw Confined Disposal Facility. J. Great Lakes Res., 19(1):158-174.

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William L. Richardson

Environmental Engineer
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7611
Fax: (734) 692-7603
wlr@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Chairperson, Modeling Workgroup. Facilitates overall development of Lake Michigan models by coordinating efforts between participating organizations and between project workgroups. Directing data management aspects of model development and participating in model development and application for atrazine and *trans*-nonachlor.

Education

B.S.E., Civil Engineering, University of Michigan, Ann Arbor, Michigan
Graduate Studies in Water Resource Engineering, University of Pennsylvania and University of Michigan.
Attended three Manhattan College Summer Institutes for Mathematical Modeling
Licensed Professional Engineer, State of Michigan

Professional Experience

Thirty-three years experience with USEPA and predecessor agencies.

Staff engineer for Delaware Estuary Comprehensive Study which was one of the first projects to use computers and systems analysis to solve water quality problems.

Research Physical Scientist for USEPA/ORD Great Lakes Research Program at Grosse Ile, Michigan.

Developed first calibrated PCB model for Saginaw Bay. Applied eutrophication model for Saginaw Bay.

Developed five lake-in-series model for Great Lakes to predict future concentrations of chloride.

Station Chief responsible for Great Lakes Research Program from 1983 to 1994.

Chairman Green Bay Mass Balance Project.

Led efforts for modeling the Detroit River, Monroe Harbor, and Flint River.

Developed MICHTOX for modeling toxic substances in rivers and streams.

Developed and prepared the report "Guidance for Waste Load Allocation of Toxic Chemicals in Rivers and Streams" as used by the Office of Water and States. Project Officer for modeling cooperative agreements which led to eutrophication, toxic chemical, and food chain models for the Great Lakes.

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Kenneth R. Rygwelski

Environmental Scientist
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7641
Fax: (734) 692-7603
krr@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Member of Modeling Worgroup. Developing and applying models for atrazine and mercury.

Education

Graduate Certificate, Hazardous Waste Control, Wayne State University, Detroit, Michigan, 1995
M.S., Chemical Engineering, Wayne State University, Detroit, Michigan, 1983
B.S., Chemistry, Michigan Technological University, Houghton, Michigan, 1972

Professional Experience

From 1995 to present - Work involves research projects including development and application of mathematical mass balance models for mercury and atrazine in Lake Michigan. Maintains an atrazine screening-level model, MICHTOX, which is a WASP-based model. This model is a precursor to a more finely segmented WASP model. Mercury modeling will likely utilize a WASP model that will take into consideration the various mercury species likely to exist. Currently, MINTEQA2, a metal speciation model is running that describes the likely composition of mercury species in Lake Michigan. MINTEQA2 will be utilized either independently of the mercury transport and fate model or incorporated within the transport and fate model. I expect to be involved in various aspects of both the atrazine and mercury modeling activities, including, model development, loading estimation, data review, model computations, and report writing. Previous experience includes managing on-site contractor staff for ADP support at the LLRS with database management responsibilities for several large USEPA projects. Before that was staff inorganic chemist responsible for analytical chemistry for heavy metals.

Publications

Book Chapters

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Rathbun, J.E., M.L. Gessner, V.E. Smith, D.M. Lemon, D.J. Brokaw, M.A. Hoeft, W.L. Richardson, and K.R. Rygwelski. 1984. Bioaccumulation to Total PCBs and PCB Homologs in Caged Clams, Channel Catfish, and Fathead Minnows in the Monroe Harbor - River Raisin, Michigan (1984). U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 74 pp.

Winfield, R.P., W.L. Richardson, M. Labiak, K. Rygwelski, D.M. Di Toro, and R. Andrews. 1983. Mathematical Models of the Fate of Pentachlorobiphenyls in an Experimental Stream. U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 31 pp.

Presentations

Endicott, D.D., W.L. Richardson, K.R. Rygwelski, X. Zhang, J.J. Pauer, and X. Zhang. 1997. Conceptual and Mathematical Models for the Lake Michigan Mass Balance Project. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Great Lakes Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Richardson, W.L., D.D. Endicott, and K.R. Rygwelski. 1997. Quality Assurance for the Lake Michigan Mass Balance Project. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Great Lakes Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Rygwelski, K.R., W.L. Richardson, and D.D. Endicott. 1997. A Screening-Level Model Evaluation of Atrazine in the Lake Michigan Basin. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Great Lakes Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Martin, J.L., M. Velleux, and K. Rygwelski. 1989. Screening-Level PCB of Model of Green Bay, Lake Michigan. 32nd Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Madison, Wisconsin. May 30-June 2, 1989.

Dolan, D.M., S.A. Megens, and K. Rygwelski. 1988. Total Phosphorus Loadings from the Detroit River to Lake Erie in 1986. 31st Conference on Great Lakes Research, International Association for Great Lakes Research, McMaster University, Hamilton, Ontario, Canada. May 16-20, 1988.

Rygwelski, K.R., J.L. Martin, W.L. Richardson, and S.L. Kleiber. 1988. Mass Budget of Toxic and Conventional Pollutants in the Trenton Channel. 31st Conference on Great Lakes Research, International Association for Great Lakes Research, McMaster University, Hamilton, Ontario, Canada. May 16-20, 1988.

Bridgham, S.D., D. McNaught, C. Meadows, K. Rygwelski, D. Dolan, and M. Gessner. 1985. Factors Responsible for the Inhibition or Stimulation of Two Great Lakes Ecosystems. 28th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Milwaukee, Wisconsin. June 3-5, 1985.

Mathews, S.H., D.M. Dolan, K.R. Rygwelski, and D. Griesmer. 1985. Correlations of Biological Effects and Metal Contaminants at Monroe Harbor, Michigan. 28th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Milwaukee, Wisconsin. June 3-5, 1985.

Richardson, W.L., K.R. Rygwelski, and R.P. Winfield. 1985. Mass Balances of Toxic Substances in an IJC Class A Area of Concern. 28th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Milwaukee, Wisconsin. June 3-5, 1985.

Winfield, R.P., W.L. Richardson, M. Labiak, K. Rygwelski, D.M. Di Toro, and R. Andrews. 1983. Mathematical Models of the Fate of Pentachlorobiphenyl in an Experimental Stream. Fourth Annual Meeting of the Society of Environmental Toxicology and Chemistry, Arlington, Virginia. November 6-9, 1983.

Rygwelski, K.R. and J.M. Townsend. 1981. Partitioning of Cadmium, Copper, Lead, and Zinc Among Water and Particulate Fractions in Saginaw Bay, Lake Huron. 24th Conference on Great Lakes Research, International Association for Great Lakes Research, The Ohio State University, Columbus, Ohio. April 28-30, 1981.

Rygwelski, K.R., J.M. Spurr, and J.M. Townsend. 1978. Necessary Quality Control for the Analysis of Trace Metals in Lake Water. 21st Conference on Great Lakes Research, International Association for Great Lakes Research, University of Windsor, Windsor, Ontario, Canada. May 9-11, 1978.

James J. Pauer

Water Quality Modeler
SoBran, Incorporated
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7635
Fax: (734) 692-7603
jjp@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Eutrophication (phytoplankton, solids) modeling.

Education

Ph.D., Environmental Engineering, Michigan Technological University, Houghton, Michigan

Training

Advanced Water Quality Modeling Short Course by Steve Chapra, 1995

QUAL2E Modeling Course by Brown and Barnwell, Athens, Georgia

Waste Load Allocation Course by Ray Whittemore, Tufts University

Experience as Related to Modeling

Three years experience in water quality modeling and impact assessment studies (CSIR, South Africa).

Publications

Pauer, J.J. 1996. Nitrification in Lake and River Systems Doctoral Thesis, Michigan Technological University, Houghton, Michigan.

Presentations

Endicott, D.D., W.L. Richardson, K.R. Rygwelski, X. Zhang, J.J. Pauer, and X. Zhang. 1997. Conceptual and Mathematical Models for the Lake Michigan Mass Balance Project. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Great Lakes Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Pauer, J.J. 1995. River Nitrification: Are Large Ranges in Reported Rate Coefficients Trying to Tell Us Something? WEFTEC '95 Conference.

Pauer, J.J. The Impact of the SAPPI Tugela Mill Effluent on Dissolved Oxygen in the Tugela River. South African Pulp and Paper Technical Conference, South Africa.

Xiaomi Zhang

Water Quality Modeler
SoBran, Incorporated
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7624
Fax: (734) 692-7603
zxm@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Responsible for general water quality model development and application. Calibrate the transport submodel by using hydrodynamic model output and adjusting WASP input so that measured temperature regimes are simulated. Responsible for implementing transport and fate submodels at various time and spatial scales and apply to PCBs, mercury, *trans*-nonachlor, and atrazine.

Education

M.S., Civil Engineering (Environmental), State University of New York at Buffalo, Buffalo, New York, 1995.
M.A., Geology (Geophysics), State University of New York at Buffalo, Buffalo, New York, 1992.
B.S., Geophysics, ChangChun GeoScience and Technology University, ChangChun, China, 1984.

Training

Oracle Training Certified, January 1997.

Experience

Environmental Engineer/Water Quality Modeler, SoBran, Incorporated, May 1995-Present

Develop, calibrate, diagnose water quality models describing toxic contaminant transport and fate in the aquatic environment. Experience with the modeling frameworks including WASP4 type models such as GBTOX, IPX etc. Work assignments and accomplishments include: writing GBTOX user's guide and Green Bay Mass Budget diagram generation guide; analysis for Lake Michigan PCB volatilization flux; Lake Michigan Level II Segmentation scheme design; IPX, GBTOX model codes modification for LMMBP; and vertical dispersion coefficients calibration for LMMBP by using those models.

Research Assistant, Great Lake Program, State University of New York at Buffalo, Buffalo, New York, 1993-May 1995

Recalibration of GBTOX model for GBMBS including both organic carbons model and toxic chemical model calibrations. Masters' thesis research focused on the effect of spatial resolution (i.e. segmentation scheme) on the biochemical transformation parameters and toxic chemical partition coefficients and long-term management diagnosis (using GBMBS generated data)

Publications

Zhang, X. and W. Richardson. 1995. GBTOX User's Guide and Green Bay Mass Budget Diagram Generation Guide. U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 57 pp.

Raghunathan, R., J. DePinto, S. Martin, V. Bierman, Jr., P. Rodgers, T. Young, and X. Zhang. 1994. Development of a Toxic Chemical Dynamics Model (GBTOX) for the Green Bay Mass Balance Study. Part 1: Model Framework and Calibration; Part 2: Model Diagnosis and Interpretation. J. Great Lakes Res., in preparation.

DePinto, J.V., R. Raghunathan, P. Sierzenga, X. Zhang, V.J. Bierman, Jr., P.W. Rodgers, and T.C. Young. 1993. Recalibration of GBTOX: An Integrated Exposure Model for Toxic Chemicals in Green Bay, Lake Michigan. Final Report. U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 132 pp.

Presentations

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Zhang, X. 1996. Relationship Between the Models of the Lake Michigan Modeling Framework and Inputs Needed for the Contaminant Mass Balance Model (the Modified IPX). Third Annual Meeting of Lake Michigan Mass Balance Project, Chicago, Illinois. December 10-12, 1996.

Xin Zhang

Ph.D., Mathematical Modeler
PAI/SoBran, Incorporated
U.S. Environmental Protection Agency
ORD, NHEERL, MED-Duluth, CBSSS, LLRS
9311 Groh Road
Grosse Ile, Michigan 48138
(734) 692-7631
Fax: (734) 692-7603
xin@lloyd.grl.epa.gov

Role in the Lake Michigan Mass Balance Project

Responsible for modeling chemical bioaccumulation in Lake Michigan food webs.

Education

Ph.D., Chemical Thermodynamics

Training

Postdoctoral training in uptake and bioaccumulation of chemical substances in fish, plants, and other organisms, modeling the dynamics of chemical distribution in aquatic ecosystem and food chains, relationships between chemical structure and environmental fate of organic compounds.

Experience

Mathematical Modeler, PAI/SoBran, Incorporated, June 1996-present

Modeling food web bioaccumulation of PCBs as a part of Lake Michigan Modeling Project.

Research Associate, Environmental Contaminants Laboratory, School of Resource and Environmental Management, Simon Fraser University, Canada, November 1991-June 1996

Several projects on modeling studies of the environmental fate and bioaccumulation of chemical contaminants in Lake Ontario, Fraser-Thompson River, and Vancouver Harbor.

Development of "Chemical Ranker" computer program for the British Columbia government to rank organic chemicals based on exposure and toxic effects to organisms.

Development of a computer program "Food-Web Bioaccumulation Model" to estimate the water and sediment concentrations associated with acceptable contaminant levels in fish. This program has been formally and favorably reviewed by the USEPA for use in its Great Lakes Water Quality Initiative (EPA-822-R-94-002).

Development of quantitative molecular structure-property relationships (QSPR) to predict physical chemical properties of a large group of organic contaminants for environmental hazard assessment.

Laboratory studies on the mechanism of bioaccumulation of organic compounds in fish (guppy, goldfish, and rainbow trout).

Publications

Gobas, F.A.P.C., M.N. Z'Graggen, and X. Zhang. 1995. Time Response of the Lake Ontario Ecosystem to Virtual Elimination of PCBs. Environ. Sci. Technol., 29(8):2038-2046.

Modeling the Environmental Fate and Food-Chain Bioaccumulation of Pulp Mill Effluent Contaminants in the Fraser-Thompson River System. 1995. Technical Report. British Columbia Ministry of the Environment, British Columbia, Canada.

Zhang, X. and F.A.P.C. Gobas. 1995. A Thermodynamic Analysis of the Relationship Between Molecular Size, Hydrophobicity, Aqueous Solubility and Octanol-Water Partitioning of Organic Chemicals. Chemosphere, 31(6):3501-3521.

Chemical Property Characterization and Chemical Exposure and Hazard Ranking of Chemicals in Pulp and Paper Mill Effluents. 1994. Technical Report. British Columbia Ministry of the Environment, British Columbia, Canada.

Gobas, F. and X. Zhang. 1994. Interactions of Organic Chemicals with Organic Matter in the Aquatic Environment. In - Jerry J. Hamelik (Ed.), Bioavailability, Physical, Chemical, and Biological Interactions. CRC Press, Inc., New York, New York.

Gobas, F.A.P.C., X. Zhang, and R. Wells. 1993. Gastrointestinal Magnification: The Mechanism of Biomagnification and Food Chain Accumulation of Chemicals. Environ. Sci. Technol., 27(12):2855-2863.

Gobas, F.A.P.C. and X. Zhang. 1992. Measuring Bioconcentration Factors and Rate Constants of Chemicals in Aquatic Organisms under Conditions of Variable Water Concentrations and Short Exposure Time. Chemosphere, 25(12):1961-1972.

Zhang, X. and L.G. Heplor. 1991. Application of Calorimetry to Investigations of Kinetics and Energetics of Oxidation of Fuels: Experimental and Calculational Methods for Initial Rates. Thermochim. Acta, 191:155-159.

Presentations

Endicott, D.D., W.L. Richardson, K.R. Rygwelsi, X. Zhang, J.J. Pauer, and X. Zhang. 1997. Conceptual and Mathematical Models for the Lake Michigan Mass Balance Project. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Zhang, X. and F.A.P.C. Gobas. 1997. A Model for the Bioaccumulation of Mercury Species in the Lake Ontario Food Web. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Zhang, X. and F.A.P.C. Gobas. 1997. A Mass Balance and Historical Contamination Profile of Mirex in Lake Ontario Ecosystem. 40th Conference on Great Lakes Research, International Association for Great Lakes Research, Center for Environmental Research and Education, Buffalo State College, Buffalo, New York. June 1-5, 1997.

Zhang, X. and FA.P.C. Gobas. 1995. ECOFATE: A User-Friendly Environmental Fate, Bioaccumulation and Ecological Risk Assessment Model for Contaminants in Marine and Freshwater Aquatic Ecosystems: Application and Validation. Second Society of Environmental Toxicology and Chemistry World Congress, Vancouver, British Columbia, Canada. November 5-9, 1995.

Wilcockson, J., F. Gobas, and X. Zhang. 1995. Biomagnification and Bioavailability of Hexachlorobiphenyl in Rainbow Trout. Second Society of Environmental Toxicology and Chemistry World Congress, Vancouver, British Columbia, Canada. November 5-9, 1995.

Gobas, F. and X. Zhang. 1994. Mechanisms and Simulation Models of Contaminant Bioconcentration and Biomagnification in Aquatic Food-Webs. Fifteenth Annual Meeting of the Society of Environmental Toxicology and Chemistry, Denver, Colorado. October 30-November 3, 1994.

Victor J. Bierman, Jr., Ph.D.

Environmental Engineering
Associate Vice-President
Limno-Tech, Incorporated
501 Avis Drive
Ann Arbor, Michigan 48108
(734) 973-8300
Fax: (734) 973-1069

Role in the Lake Michigan Mass Balance Project

Direct the conceptualization and development of the ecosystem model. Provide expert advice regarding model construct, principles, testing, and parameter refinements.

Education

Ph.D., Environmental Engineering, University of Notre Dame, Notre Dame, Indiana, 1974
M.S., Physics, University of Notre Dame, Notre Dame, Indiana, 1971
A.B., Science, Villanova University, Vallanova, Pennsylvania, 1966

Specialized Training and Coursework

Institute on Mathematical Modeling of Water Quality, Manhattan College, Bronx, New York, 1985

Professional Experience

Associate Vice-President, Limno-Tech, Inc., Ann Arbor, Michigan, 1997.

Senior Scientist, Limno-Tech, Inc., South Bend, Indiana, 1992-1997.

Senior Project Manager, Limno-Tech, Inc., South Bend, Indiana, 1990-1992.

Adjunct Associate Professor, Department of Civil Engineering and Geological Sciences, University of Notre Dame, Notre Dame, Indiana, 1990-1992.

Associate Professor, Department of Civil Engineering, University of Notre Dame, Notre Dame, Indiana, 1990-1992.

Environmental Scientist, USEPA National Expert in Environmental Exposure Assessment, Environmental Research Laboratory, USEPA, Narragansett, Rhode Island, 1981-1986.

Adjunct Associate Professor, Department of Civil and Environmental Engineering, University of Rhode Island, Kingston, Rhode Island, 1985-1986.

Environmental Scientist, USEPA, LLRS, Grosse Ile, Michigan, 1974-1981.

Systems Ecologist, Cranbrook Institute of Science, Bloomfield Hills, Michigan, 1974.

Publications

Journal Articles

DePinto, J.V., R. Raghunathan, V.J. Bierman, Jr., P.W. Rodgers, S.C. Hinz, and T.C. Young. 1995. Development and Calibration of an Organic Carbon Based Sorbent Dynamics Model (GBOCS) for the Green Bay Mass Balance Study. Submitted for publication in the Journal of Great Lakes Research.

DePinto, J.V., P. Sierzenga, R. Raghunathan, V.J. Bierman, Jr., P.W. Rodgers, S.C. Hinz, and T.C. Young. 1995. Vertical Dynamics of Particulate Matter in Green Bay: A Long-Term Radionuclide (^{137}Cs) Mass Balance Model. Submitted for publication in the Journal of Great Lakes Research.

Havens, K.E., V.J. Bierman, Jr., E.G. Flaig, C. Hanlon, R.T. James, B.L. Jones, and V.H. Smith. 1995. Historical Trends in the Lake Okeechobee Ecosystem, VI, Synthesis. Archiv. Hydrobiol., Supplement, 107:101-111.

James, R.T. and V.J. Bierman, Jr. 1995. A Preliminary Modeling Analysis of Water Quality in Lake Okeechobee, Florida: Calibration Results. Water Res., 29(12):2767-2775.

Martin, S.C., S.C. Hinz, P.W. Rodgers, V.J. Bierman, Jr., J.V. DePinto, and T.C. Young. 1995. Calibration of a Hydraulic Transport Model for Green Bay, Lake Michigan. J. Great Lakes Res., 21(4):599-609.

Raghunathan, R., J.V. DePinto, S.C. Martin, V.J. Bierman, Jr., P.W. Rodgers, T.C. Young, and X. Zhang. 1995. Development of a Toxic Chemical Dynamics Model (GBTOX) for the Green Bay Mass Balance Study: Part One - Model Framework and Calibration. Submitted for publication in the Journal of Great Lakes Research.

Raghunathan, R., J.V. DePinto, S.C. Martin, V.J. Bierman, Jr., P.W. Rodgers, T.C. Young, and X. Zhang. 1995. Development of a Toxic Chemical Dynamics Model (GBTOX) for the Green Bay Mass Balance Study: Part Two - Model Diagnostic Application. Submitted for publication in the Journal of Great Lakes Research.

Smith, V.H., V.J. Bierman, Jr., B.L. Jones, and K.E. Havens. 1995. Historical Trends in the Lake Okeechobee Ecosystem, IV. Nitrogen:Phosphorus Ratios, Cyanobacterial Dominance, and Nitrogen Fixation Potential. Arch. Hydrobiol., Supplement, 107:71-88.

Young, T.C., V.J. Bierman, Jr., J.V. DePinto, and P.W. Rodgers. 1995. Uncertainty of Fluvial Load Estimates From the Upper Fox River During the Green Bay Mass Balance Study. Submitted for publication in the Journal of Great Lakes Research.

Bierman, V.J., Jr., S.C. Hinz, D. Zhu, W.J. Wiseman, Jr., N.N. Rabalais, and R.E. Turner. 1994. A Preliminary Mass Balance Model of Primary Productivity and Dissolved Oxygen in the Mississippi River Plume/Inner Gulf Shelf Region. Estuaries, 17(4):886-899.

DePinto, J.V., R. Raghunathan, V.J. Bierman, Jr., P.W. Rodgers, T.C. Young, and S.C. Martin. 1993. Analysis of Organic Carbon Sediment-Water Exchange in Green Bay, Lake Michigan. Water Sci. Technol., 28(8-9):149-159.

Dilks, D.W., J.S. Helfand, V.J. Bierman, Jr., and L. Burkhard. 1993. Field Application of a Steady-State Mass Balance Model for Hydrophobic Organic Chemicals in an Estuarine System. Water Sci. Technol., 28(8-9):263-271.

Bonner, J.S., C.D. Hunt, J.F. Paul, and V.J. Bierman, Jr. 1992. Transport of Low-Level Radioactive Soil at Deep-Ocean Disposal Sites. J. Environ. Engin., 118(1):101-119.

Preston, S.D., V.J. Bierman, Jr., and S.E. Silliman. 1992. Impact of Flow Variability on Error in the Estimation of Tributary Mass Loads. J. Environ. Engin., 118(3):402-419.

Bierman, V.J., Jr. 1990. Equilibrium Partitioning and Biomagnification of Organic Chemicals in Benthic Animals. Environ. Sci. Technol., 24(9):1407-1412.

Preston, S.D., V.J. Bierman, Jr., and S.E. Silliman. 1989. An Evaluation of Methods for the Estimation of Tributary Mass Loads. Water Resources Res., 25(6):1379-1389.

Walker, H.A., J.F. Paul, and V.J. Bierman, Jr. 1987. Methods for Waste Load Allocation of Municipal Sewage Sludge at the 106-Mile Ocean Disposal Site. Environ. Toxicol. Chem., 6(6):475-489.

Bierman, V.J., Jr. and D.M. Dolan. 1986. Modeling of Phytoplankton in Saginaw Bay: I. Calibration Phase. J. Environ. Engin., 112(2):400-414.

Bierman, V.J., Jr. and D.M. Dolan. 1986. Modeling of Phytoplankton in Saginaw Bay: II. Post-Audit Phase. J. Environ. Engin., 112(2):415-429.

O'Connor, T.P., H.A. Walker, J.F. Paul, and V.J. Bierman, Jr. 1985. A Strategy for Monitoring of Contaminant Distributions Resulting From Proposed Sewage Sludge Disposal at the 106-Mile Ocean Disposal Site. Marine Environ. Res., 16:127-150.

Bierman, V.J., Jr., D.M. Dolan, R. Kasprzyk, and J.L. Clark. 1984. Retrospective Analysis of the Response of Saginaw Bay, Lake Huron, to Reductions in Phosphorus Loadings. Environ. Sci. Technol., 18(1):23-31.

Bierman, V.J., Jr. and W.R. Swain. 1982. Mass Balance Modeling of DDT Dynamics in Lakes Michigan and Superior. Environ. Sci. Technol., 16(9):572-579.

Dolan, D.M. and V.J. Bierman, Jr. 1982. Mass Balance Modeling of Heavy Metals in Saginaw Bay, Lake Huron. J. Great Lakes Res., 8(4):676-694.

Bierman, V.J., Jr. and D.M. Dolan. 1981. Modeling of Phytoplankton-Nutrient Dynamics in Saginaw Bay, Lake Huron. J. Great Lakes Res., 7(4):409-439.

Dolan, D.M., V.J. Bierman, Jr., M.H. Dipert, and R.D. Geist. 1978. Statistical Analysis of the Spatial and Temporal Variability of the Ratio Chlorophyll *a* to Phytoplankton Cell Volume in Saginaw Bay, Lake Huron. J. Great Lakes Res., 4(1):75-83.

Refereed Book Chapters

Bierman, V.J., Jr. 1993. Partitioning of Organic Chemicals in Sediments: Estimation of Interstitial Concentrations Using Organism Body Burdens. In - J.V. DePinto, W. Lick, and J.F. Paul (Eds.), Transport and Transformation of Contaminants Near the Sediment-Water Interface, pp. 149-170. Lewis Publishers, Chelsea, Michigan.

Walker, H.A., J.F. Paul, and V.J. Bierman, Jr. 1990. A Convective-Dispersive Transport Model for Wastes Disposed at the 106-Mile Ocean Disposal Site. In - D.J. Baumgartner and L.W. Duedall (Eds.), Oceanic Processes in Marine Pollution, Volume 6 - Physical and Chemical Processes: Transport and Transformation, pp. 53-61. Krieger, Malabar, Florida.

Gentile, J.H., V.J. Bierman, Jr., J.F. Paul, H.A. Walker, and D.C. Miller. 1989. A Hazard Assessment Research Strategy for Ocean Disposal. In - M.A. Champ and P.K. Park (Eds.), Oceanic Processes in Marine Pollution, Volume 3 - Marine Waste Management: Science and Policy, pp. 200-212. Krieger, Malabar, Florida.

Paul, J.F., V.J. Bierman, Jr., H.A. Walker, and J.H. Gentile. 1989. Application of a Hazard Assessment Research Strategy for Waste Disposal at the 106-Mile Ocean Disposal Site. In - D.W. Hood, A. Schoener, and P.K. Park (Eds.), Oceanic Processes in Marine Pollution, Volume 4 - Scientific Monitoring Strategies for Ocean Waste Disposal, pp. 149-160. Krieger, Malabar, Florida.

Reed, M. and V.J. Bierman, Jr. 1989. A Protocol for Designation of Ocean Disposal Sites. In - M.A. Champ and P.K. Park (Eds.), Oceanic Processes in Marine Pollution, Volume 3 - Marine Waste Management: Science and Policy, pp. 155-166. Krieger, Malabar, Florida.

Paul, J.F., V.J. Bierman, Jr., W.R. Davis, G.L. Hoffman, W.R. Munns, C.E. Pesch, P.F. Rogerson, and S.C. Schimmel. 1988. The Application of a Hazard Assessment Research Strategy to the Ocean Disposal of a Dredged Material: Exposure Assessment Component. In - D.A. Wolfe and T.P. O'Connor (Eds.), Oceanic Processes in Marine Pollution, Volume 5 - Urban Wastes in Coastal Marine Environments, pp. 123-135. Krieger, Malabar, Florida.

Bierman, V.J., Jr., J.H. Gentile, J.F. Paul, D.C. Miller, and W.A. Brungs. 1986. Research Strategy for Ocean Disposal: Conceptual Framework and Case Study. In - H.L. Bergman, R.A. Kimerle, and A.W. Maki (Eds.), Environmental Hazard Assessment of Effluents, pp. 313-329. Pergamon Press, New York, New York.

Bierman, V.J., Jr. 1976. Mathematical Model of the Selective Enhancement of Blue-Green Algae by Nutrient Enrichment. In - R.P. Canale (Ed.), Modeling Biochemical Processes in Aquatic Ecosystems, pp. 1-31. Ann Arbor Science Publishers, Ann Arbor, Michigan.

DePinto, J.V., V.J. Bierman, Jr., and F.H. Verhoff. 1976. Seasonal Phytoplankton Succession as a Function of Phosphorus and Nitrogen Levels. In - R.P. Canale (Ed.), Modeling Biochemical Processes in Aquatic Ecosystems, pp. 141-169. Ann Arbor Science Press, Ann Arbor, Michigan.

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Preston, S.D., V.J. Bierman, Jr., and S.E. Silliman. 1989. Evaluation of Methods for the Estimation of Tributary Mass Loading Rates. U.S. Geological Survey, Water Resources Research Center, Purdue University, West Lafayette, Indiana. Technical Report No. 187, 50 pp.

Bierman, V.J., Jr., S.D. Preston, and S.E. Silliman. 1988. Development of Estimation Methods for Tributary Loading Rates of Toxic Chemicals. U.S. Geological Survey, Water Resources Research Center, Purdue University, West Lafayette, Indiana. Technical Report No. 183, 58 pp.

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Dolan, D.M., V.J. Bierman, Jr. and R.D. Geist. 1978. Dynamic Mass Balance for Cadmium and Zinc in Saginaw Bay, Lake Huron. 21st Conference on Great Lakes Research, International Association for Great Lakes Research, University of Windsor, Windsor, Ontario, Canada.

Bierman, V.J., Jr. and D.M. Dolan. 1977. Mathematical Modeling of Phytoplankton Growth Kinetics as a Function of Multiple Nutrient Limitation. 20th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Michigan, Ann Arbor, Michigan.

Bierman, V.J., Jr., W.L. Richardson, and D.M. Dolan. 1976. A Multi-Class Model of Phytoplankton Production in Saginaw Bay, Lake Huron. 19th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Guelph, Guelph, Ontario, Canada.

Richardson, W.L. and V.J. Bierman, Jr. 1975. A Time-Variable Model of Chloride Distribution in Saginaw Bay, Lake Huron. 18th Conference on Great Lakes Research, International Association for Great Lakes Research, State University of New York, Albany, New York. May 20-23, 1975.

Bierman, V.J., Jr. 1974. Dynamic Mathematical Model of Algal Growth and Species Competition for Phosphorus, Nitrogen and Silica. 17th Conference on Great Lakes Research, International Association for Great Lakes Research, McMaster University, Hamilton, Ontario, Canada. August 12-14, 1974.

Client Reports

Everglades Water Quality Model Calibration Report. Prepared for South Florida Water Management District, West Palm Beach, Florida. 1997.

Application of a Coupled Primary Productivity-Exotic Species Model for Saginaw Bay, Lake Huron. Prepared for the U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 1997.

Estimated Responses of Water Quality on the Louisiana Inner Shelf to Nutrient Load Reductions in the Mississippi and Atchafalaya Rivers. Prepared for the U.S. Environmental Protection Agency, Gulf of Mexico Program Office, Stennis Space Center, Mississippi. 1995.

A Preliminary Ecosystem Modeling Study of Zebra Mussels (*Dreissena polymorpha*) in Saginaw Bay, Lake Huron. Prepared for the U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. 1995.

Preliminary Assessment of Nitrogen Impacts on the Lake Okeechobee Ecosystem. Prepared for the South Florida Water Management District, West Palm Beach, Florida. 1993.

Evaluation of Nitrogen Removal Eutrophication Risk for the Freshwater Potomac Estuary. Prepared for Metropolitan Washington Council of Governments, Washington, D.C. 1993.

Phase II Screening Model Application to Dioxin (2,3,7,8-TCDD) in the Columbia River. Prepared for the U.S. Environmental Protection Agency, Region X, Seattle, Washington. 1992.

Screening Level Analysis for Estimation of Sediment Quality Criteria Impacts. Prepared for the Office of Wastewater Enforcement and Compliance, U.S. Environmental Protection Agency, Washington, D.C. 1992.

Timothy J. Feist
Environmental Scientist
Limno-Tech, Incorporated
501 Avis Drive
Ann Arbor, Michigan 48108
(734) 973-8300
Fax: (734) 973-1069

Role in the Lake Michigan Mass Balance Project

Assessment of ecosystem model constructs, selection of the most appropriate model, and conceptual refinement and development of additional trophic levels in the model.

Education

M.S., Fisheries and Wildlife (Limnology), Michigan State University, East Lansing, Michigan, 1988
B.S., Fisheries and Wildlife, Michigan State University, East Lansing, Michigan, 1985

Specialized Training and Coursework

Mathematical Modeling of Water Quality: Dissolved Oxygen-Eutrophication, Manhattan College, Riverdale, New York, June 1992.

Professional Experience

Environmental Scientist, LTI-Limno-Tech, Inc., Ann Arbor, Michigan. 1990-Present.

Field Research Technician, Michigan State University, East Lansing, Michigan. 1988-1990.

Student Assistant, Michigan Department of Natural Resources, Lansing, Michigan, 1988.

Publications

Journal Articles

DeVault, D.S., R. Hesselberg, P.W. Rodgers, and T.J. Feist. 1996. Contaminant Trends in Lake Trout and Walleye From the Laurentian Great Lakes. J. Great Lakes Res., 22(4):884-895.

Feist, T.J. and N.R. Kevern. 1989. Nutrient Study of a New Reservoir, Sessions Lake, Michigan. Mich. Academ., 21(4):339-358.

Presentations and Symposiums

Bierman, V.J., Jr., D.W. Dilks, T.J. Feist, J.V. DePinto, and R.G. Kreis, Jr. 1997. Mass Balance Modeling of Zebra Mussel, Blue-Green Phytoplankton and Phosphorus Dynamics in Saginaw Bay, Lake Huron. Seventh International Zebra Mussel and Aquatic Nuisance Species Conference, New Orleans, Louisiana. January 28-31, 1997.

Bierman, V.J., Jr., D.W. Dilks, T.J. Feist, and J.V. DePinto. 1996. A Mass Balance Analysis of Relationships Among Zebra Mussels, Blue-Green Phytoplankton and Sediment Phosphorus Flux in Saginaw Bay, Lake Huron. 39th Conference on Great Lakes Research, International Association for Great Lakes Research, Erindale College, University of Toronto, Mississauga, Ontario, Canada. May 26-30, 1996

Feist, T.J., C.E. Mericas, C.T. Cieciek, P. Adriaens, and A. Barkovskii. November 1996. Evaluation of Aeration and Bioaugmentation for Decreasing Sediment Thickness in Austin Lake, Michigan. Sixteenth Annual International Symposium on the North American Lake Management Society.

Encouraging Science-Based Lake Management: What is Needed in a Comprehensive Lake Management Plan. Panel Presentation - Lake Management in Michigan: A Call to Action Workshop, Michigan Chapter North American Lake Management Society. March 1996.

Dilks, D.W., V.J. Bierman, Jr., T.J. Feist, and D.E. Maricas. November 1994. Use of Models in Assessing Exotic Species: A Zebra Mussel Example. Fourteenth International Conference of the North American Lake Management Society, Orlando, Florida.

Feist, T.J., T.A.D. Slawecki, and D.e. Mericas. November 1994. Evaluating Watershed Impacts on Waterbodies Using GIS. Fourteenth International Conference of the North American Lake Management Society, Orlando, Florida.

DePinto, V.J., P.W. Rodgers, and T.J. Feist. June 1994. When Do Sediment-Water Interactions Control the Water Column Response of Large Lakes to Toxic Chemical Load Reductions? 37th Conference on Great Lakes Research, International Association for Great Lakes Research, University of Windsor, Windsor, Ontario, Canada. June 5-9, 1994.

Feist, T.J., V.J. Bierman, Jr., and L. Beasley. June 1993. Trend Analysis of Saginaw River Phosphorus Loads, 1981-1990. 36th Conference on Great Lakes Research, International Association for Great Lakes Research, St. Norbert College, DePere, Wisconsin. June 4-10, 1993.

Rodgers, P.W. and T.J. Feist. February 1993. Watershed Management of Nutrients. Innovations in Water and Wastewater Seminar in the 90's, University of Michigan, Ann Arbor, Michigan.

Client Reports

Evaluation of Aeration and Bioaugmentation for Decreasing Sediment Thickness in Austin Lake. Project report for the City of Portage, Michigan, January 1996.

First and Second Sister Lakes Diagnostic/Feasibility Study. Project report for the City of Ann Arbor Department of Parks and Recreation, Ann Arbor, Michigan, September 1995.

Interim Data Review Report. Project report for the South Florida Water Management District, West Palm Beach, Florida, March 1995.

A Preliminary Ecosystem Modeling Study of Zebra Mussels (*Dreissena polymorpha*) in Saginaw Bay, Lake Huron. Report to the U.S. Environmental Protection Agency, Office of Research and Development, ERL-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. February 1995.

Higgins Lake Septic System and Lawn Fertilizer Management Zones. Project report for the Higgins Lake Foundation, Higgins Lake, Michigan, February 1994.

Higgins Lake Clean Lakes Study Pollution Control Plan. Project report for Gerrish and Lyon Townships, Roscommon County, Michigan, December 1992.

Impacts of the Greenaway Drain on Wolverine Lake, Phase II Report. Project report for the Village of Wolverine Lake, Michigan, September 1992.

Higgins Lake Diagnostic and Feasibility Study. Project report for Gerrish and Lyon Townships, Roscommon County, Michigan, May 1992.

Septic System Phosphorus Loadings to Higgins Lake, Michigan. Project report for the Higgins Lake Foundation, Higgins Lake, Michigan, February 1992.

Dissolved Oxygen Monitoring of Higgins Lake - 1991. Project report for the Higgins Lake Foundation, Higgins Lake, Michigan, January 1992.

Evaluation of Potential Impacts on Juday Creek from Proposed Detention Basins. Project report for the St. Joseph County Drainage Board, South Bend, Indiana, October 1991.

Impacts of Greenaway Drain on Wolverine Lake, Phase I Report. Project report for the Village of Wolverine Lake, Michigan, June 1990.

Effects of Artificial Destratification on Selected Water Quality Parameters and Biota of Mud Lake, Oakland County, Michigan. Batterson, T.R., R.S. Beebe and T.J. Feist. Project report for Kobe Steel Ltd., Tokyo, Japan, March 1989.

Scott C. Hinz

Senior Environmental Engineer
Limno-Tech, Incorporated
501 Avis Drive
Ann Arbor, Michigan 48108
(734) 973-8300
Fax: (734) 973-1069

Role in the Lake Michigan Mass Balance Project

Responsible for reviewing eutrophication models, coordination of ecosystem model construct revisions, expert evaluation of data input requirements, source code for the ecosystem model, and model documentation.

Principal Expertise

Water Quality Modeling
Mathematical Model Development
Hydraulics/Hydrology
Computer Programming
Estuarine Assessment
Urban Nonpoint Source Pollution
Mixing Zone/NPDES Issues
Stormwater/Sewer Modeling

Education

M.S.E., Environmental Engineering, The University of Michigan, Ann Arbor, Michigan, 1985.
B.S.E., Environmental Sciences Engineering, The University of Michigan, Ann Arbor, Michigan, 1982.

Specialized Training and Coursework

Total Quality Improvement Training. Delta Systems and LTI, Limno-Tech, Inc., Ann Arbor, Michigan, April-May 1993.

Total Quality Awareness Seminar. Ann Arbor Consulting Association, Inc. and LTI, Limno-Tech, Inc., Ann Arbor, Michigan, September 1992.

Technical Writing Seminar. The University of Michigan, College of Engineering and LTI, Limno-Tech, Inc., Ann Arbor, Michigan, February 1992.

Project Management Course. LTI, Limno-Tech, Inc., Ann Arbor, Michigan, May-July 1990.

Experience Summary

Mr. Hinz has 16 years of experience in developing and applying water quality, hydrologic, and hydrodynamic models to systems throughout the United States. His particular expertise and training is in the areas of water quality and hydrologic assessments of natural systems. Mr. Hinz is conversant in a wide range of programming languages and is familiar with main-frame and microcomputer systems. As a Senior Environmental Engineer with Limno-Tech, Mr. Hinz has developed and applied water quality models to evaluate toxic organic chemicals, metals, eutrophication, and dissolved oxygen problems. His major role at Limno-Tech is providing advice, support, and technical review of complex water quality modeling applications.

Mr. Hinz's work has included extensive enhancements to USEPA's WASP4 and WASP5 toxics and eutrophication models to simulate water quality on a wide range of water bodies, including lakes, estuaries, and near-coastal zones. He has also developed and applied finite element hydrodynamic and water quality models for evaluating toxic mixing zones in riverine and estuarine situations, as well as standard USEPA-supported dilution models, such as the CORMIX expert system software. In the area of wet weather assessments, Mr. Hinz has developed software for evaluating historical precipitation data and applied runoff and sewer models (USEPA SWMM and the Limno-Tech's own SOM models) to evaluate best management practices for controlling wet weather discharges.

Professional Experience

Senior Environmental Engineer, Limno-Tech, Inc., Ann Arbor, Michigan, 1988-Present.

Project Engineer, Limno-Tech, Inc., Ann Arbor, Michigan. 1982-1987.

Professional Affiliations

Water Environment Federation, 1993-Present
Michigan Water Environment Association, 1993-Present

New England Water Environment Association, 1996-Present
International Association for Great Lakes Research, 1990-Present

Publications

Journal Articles

Martin, S.C., S.C. Hinz, P.W. Rodgers, V.J. Bierman, Jr., J. DePinto, and T.C. Young. 1995. Calibration of a Hydraulic Model for Green Bay, Lake Michigan. J. Great Lakes Res., 21(4):599-609.

DePinto, J.V., R.K. Raghunathan, V.J. Bierman, Jr., P.W. Rodgers, S.C. Hinz, and T.C. Young. 1995. Development and Calibration of an Organic Carbon Based Sorbent Dynamics Model (GBOCS) for the Green Bay Mass Balance Study. Submitted to the Journal of Great Lakes Research.

Bierman, V.J., Jr., S.C. Hinz, D.W. Zhu, W.J. Wiseman, Jr., N.N. Rabalais, and R.E. Turner. 1994. A Preliminary Mass Balance Model of Primary Productivity and Dissolved Oxygen in the Mississippi River Plume/Inner Gulf Shelf Region. Estuaries, 17(4):886-899.

Presentations and Symposiums

Hinz, S.C., T.J. Fikslin, T.A.D. Slawecki, and D.W. Dilks. 1994. A Simplified Approach for Establishing Acute Mixing Zones in Tidal. Water Environment Federation 67th Annual Conference and Exposition, Chicago, Illinois. October 15-19, 1994.

Bierman, V.J., Jr., S.C. Hinz, W.J. Wiseman, Jr., N.N. Rabalais, and R.E. Turner. 1992. Mass Balance Modeling of Primary Production and Dissolved Oxygen Dynamics in the Mississippi River Plume/Inner Gulf Shelf Region. American Geophysical Union (AGU) Ocean Sciences Meeting, New Orleans, Louisiana. January 27-31, 1992.

DePinto, J.V., R.K. Raghunathan, T. Young, V.J. Bierman, Jr., and S.C. Hinz. 1991. Development and Calibration of an Organic Carbon-based Sorbent Model for Toxic Chemicals in Green Bay. 34th Conference on Great Lakes Research, International Association of Great Lakes Research, State University of New York at Buffalo, Buffalo, New York. June 3-6, 1991.

Weinle, M.E., V.J. Bierman, Jr., S.C. Hinz, and T.C. Young. 1990. Mass Balance Modeling of Organic Carbon Dynamics in Green Bay, Lake Michigan. 33rd Conference on Great Lakes Research, International Association for Great Lakes Research, University of Windsor, Windsor, Ontario, Canada. May 13-17, 1990.

Hinz, S.C., P.L. Freedman, and M.P. Sullivan. 1989. Modeling Total Residual Chlorine in the Upper Potomac Estuary. Estuarine and Coastal Modeling Conference, American Society of Civil Engineers, Newport, Rhode Island. November 1989.

Rodgers, P.W., S. Hinz, V.J. Bierman, Jr., J.V. DePinto, and T.C. Young. 1989. WASP4 Transport Development and Application to Green Bay, Wisconsin. 32nd Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Madison, Wisconsin. May 30-June 2, 1989.

Dilks, D.W. and S.C. Hinz. 1988. Dilution Modeling to Define Toxic Impairment in 93 U.S. Estuaries. 61st Annual Conference of the Water Pollution Control Federation, Dallas, Texas. October 1988.

Published Proceedings

Hinz, S.C., T.J. Fikslin, T.A.D. Slawecki and D.W. Dilks. 1994. A Simplified Approach for Establishing Acute Mixing Zones in Tidal Waters. In - Surface Water Quality and Ecology, Volume 4: Proceedings of the Water Environment Federation 67th Annual Conference and Exposition, Chicago, Illinois. October 15-19, 1994.

Bierman, Jr., V.J., S.C. Hinz, D. Zhu, W.J. Wiseman, Jr., N.N. Rabalais and R.E. Turner. 1994. Mass Balance Modeling of the Impacts of Nutrient Load Reductions in the Mississippi River on Water Quality in the Northern Gulf of Mexico. In - Surface Water Quality and Ecology, Volume 4: Proceedings of the Water Environment Federation 67th Annual Conference and Exposition, Chicago, Illinois. October 15-19, 1994.

Bierman, V.J., Jr., S.C. Hinz, W.J. Wiseman, Jr., N.N. Rabalais and R.E. Turner. 1992. Mass Balance Modeling of Water Quality Constituents in the Mississippi River Plume/Inner Gulf Shelf Region. In - Nutrient Enhanced Coastal Ocean Productivity: Proceedings of the NECOP Synthesis Workshop, National Oceanic and Atmospheric Administration, Chauvin, Louisiana. October 2-4, 1991.

Hinz, S.C., N. Katopodes, P. Freedman, M. Sullivan, and S. Freudberg. 1990. Modeling Residual Chlorine in The Potomac Estuary. In - Estuarine and Coastal Modeling: Proceedings of the 1989 American Society of Civil Engineers, Estuarine and Coastal Circulation and Pollution Transport Model Data Comparison Specialty Conference, Newport, Rhode Island.

Client Reports

Phase 2 Preliminary Model Calibration Report - Hudson River PCB Reassessment RI/FS. September 1996. Final report to U.S. Environmental Protection Agency, Region II, ARCS. Prepared for TAMS Consultants, Inc., New York, New York.

Preliminary Water Quality Assessment (of CSO-Related Water Quality Effects in the Ohio River, Licking River, and Banklick Creek). October 1996. Sanitation District No. 1 of Campbell and Kenton Counties, Kentucky.

Mixing Zone Evaluation of Discharges to the Ohio River, for Weirton Steel Corporation. 1995. Weirton, West Virginia.

Phase 2 Preliminary Model Calibration Report - Hudson River PCB Reassessment RI/FS. June 1995. Draft report to U.S. Environmental Protection Agency, Region II, ARCS. Prepared for TAMS Consultants, Inc., New York, New York.

Tidal CORMIX Development and Application to Twenty Candidate Discharge Sites in the Delaware Estuary. May 1995. Draft report for the Delaware River Basin Commission, West Trenton, New Jersey.

Development and Validation of an Integrated Exposure Model for Toxic Chemicals in Green Bay, Lake Michigan. August 1992. Final report to U.S. Environmental Protection Agency, Region V and the Great Lakes National Program Office, Chicago, Illinois.

AARA Thermal Discharge Simulations to Meet NYDEC Requirements. May 1992. Report to Foster Wheeler Enviresponse, Inc.

Modeling Mixing Zone Impacts of Intermittent Blue Plains Wastewater Chlorine Discharges. April 1992. Technical report for Greeley & Hansen Engineering, Camp Springs, Maryland and the Metropolitan Washington Council of Governments, Washington, D.C.

Predicted Dilution of the South Coastal Outfall Plume: An Application of the CORMIX2 Mixing Zone Model. February 1992. Technical report for CABE Associates, Inc., Dover, Delaware.

Model-Based Estimates of Washington, D.C. Combined Sewer Overflows to the Anacostia River. September 1990. Technical report for the Metropolitan Washington Council of Governments, Washington, D.C.

Analysis of Mixing Characteristics of Preliminary ARRA Diffuser Design. July 1990. Technical report for O'Brien and Gere Engineers, Syracuse, New York.

Development and Validation of an Integrated Exposure Model for Toxic Chemicals in Green Bay, Lake Michigan. March 1990. Two-year progress report to U.S. Environmental Protection Agency, Region V and Great Lakes National Program Office, Chicago, Illinois.

Development of a Water Quality Model for the Amelia River. September 1988. Technical report for the U.S. Environmental Protection, Region IV and Office of Water Enforcement and Permits, Washington, D.C.

Estuarine Dilution Analyses to Estimate Toxic Substance Impairment for 304(l) Identification. March 1988. Technical report for the U.S. Environmental Protection Agency, Office of Marine and Estuarine Protection and Office of Water Regulation and Standards, Washington, D.C.

Summary Report: Potomac River Residual Chlorine Study. January 1988. Technical report for the D.C. Department of Consumer and Regulatory Affairs and the Metropolitan Washington Council of Governments, Washington, D.C.

Evaluation of Critical Conditions for Assessing the Benefits of Increased Nitrification Treatment in Upper Potomac Estuary. December 1987. Technical report for the Metropolitan Washington Council of Government, Washington, D.C.

Dissolved Oxygen Predictions for Alternative Wastewater Treatment Scenarios in the Upper Potomac Estuary. September 1987. Technical report for the Metropolitan Washington Council of Government, Washington, D.C.

Validation of DEM to 1985 and 1986 Data. August 11, 1987. Technical report for the Metropolitan Washington Council of Governments, Washington, D.C.

Review of the Waste Load Allocations for the Lower Potomac and Little Hunting Creek Wastewater Treatment Plants. July 1986. Technical report for Fairfax County, Virginia.

Detroit River Plume Monitoring and Modeling Program. March 1986. Technical report by Environmental Science and Engineering, Inc., Gainesville, Florida; Limno-Tech, Inc., Ann Arbor, Michigan; and Rama Rao and Alfred, Inc., Detroit, Michigan (Report No. ESE 84-536-0542), for the Detroit Water and Sewerage Department.

Water Quality Modeling and Analysis of Gunston Cove. August 1985. Technical report for Fairfax County, Virginia.

Projected Impacts of Lower Potomac Pollution Control Plant on Gunston Cove Water Quality. December 1984. Technical report Fairfax County, Virginia.

Methodology Recommendation for the Assessment of Combined Sewer Overflow Impacts on Nearshore Lake Water Quality in the Vicinity of Indiana Harbor. October 1984. Technical report for ESEI and U.S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois.

A Waste Load Allocation for the Natchitoches and Natchez Municipal Wastewater Treatment Facilities. 1984. Technical report for the Louisiana Department of Natural Resources, Baton Rouge, Louisiana.

Workshops/Short Courses

Green Bay Mass Balance Study Workshop. U.S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois. Held in Green Bay, Wisconsin, May 24-25, 1993.

Balancing The Bay Workshop: Implications of the Green Bay/Fox River Mass Balance Study. U.S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois. Held in Chicago, Illinois, May 24-25, 1993.

Estuarine Wasteload Allocation Workshop. U.S. Environmental Protection Agency, Office of Research and Development, Athens, Georgia and LTI, Limno-Tech, Inc., Ann Arbor, Michigan. Held in Danvers, Massachusetts, November 7-9, 1989.

Orren Russell Bullock, Jr.

Meteorologist
National Oceanic and Atmospheric Administration
ERL/ARL, Atmospheric Modeling Division
EPA Mail Drop 80
Research Triangle Park, North Carolina 27711
(919) 541-1349

Role in the Lake Michigan Mass Balance Project

Primarily an advisory role on atmospheric modeling aspects of the project. Help determine approaches and solutions and review results.

Education and Training

B.S., Meteorology, North Carolina State University, 1980
M.S., Meteorology, North Carolina State University, 1984

Professional Experience

Meteorologist, NOAA, 1989-Present

Computer Programmer/Analyst, NOAA, 1987-1989

Senior Scientific Specialist, Program Resources, Inc. and Computer Sciences Corporation, 1986-1987

Technical Specialist, Computer Sciences Corporation, 1984-1986

Senior Member of the Technical Staff, Computer Data Systems, Inc., 1983-1984

Professional

American Meteorological Society (National and Local)
Secretary of Local Chapter, 1987-1988
Chairman of Local Chapter, 1991-1992
Phi Kappa Phi (Honorary Academic Society)

Publications

Bullock, O.R., Jr. 1997. Lagrangian Modeling of Mercury Air Emission, Transport and Deposition: An Analysis of Model Sensitivity to Emissions Uncertainty. Sci. Total Environ., accepted for publication.

Bullock, O.R., Jr., W.G. Benjey, and M.H. Keating. 1997. The Modeling of Regional-Scale Atmospheric Mercury Transport and Deposition Using RELMAP. Environ. Toxicol. Chem., in press.

Ching, J.K.S., E.S. Binkowski, and O.R. Bullock, Jr. 1997. Deposition of Semi-Volatile Air Toxic Pollutants to the Great Lakes: A Regional Modeling Approach. Environ. Toxicol. Chem., in press.

Bullock, O.R., Jr. 1994. A Computationally Efficient Method for the Characterization of Sub-Grid-Scale Precipitation Variability for Sulfur Wet Removal Estimates. Atmos. Environ., 28:555-566.

Bullock, O.R., Jr., S.J. Roselle, and W.E. Heilman. 1989. Development and Preliminary Testing of a First-Generation Regional Aerosol Model. Internal Report. U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

Clark, T.L., O.R. Bullock, Jr., and S.J. Roselle. 1989. Simulating Regional Visibility Using an Eulerian Aerosol Model. Internal Report. U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

Presentations

Bullock, O.R., Jr. 1996. Lagrangian Modeling of Mercury Air Emission, Transport and Deposition with Source-Type Discrimination. Fourth International Conference on Mercury as a Global Pollutant, Hamburg, Germany. August 4-8, 1996.

Bullock, O.R., Jr. 1993. Evaluation of MM4/FDDA Simulations Using Independent Observations of Wind, Temperature and Humidity. Third Penn State/NCAR Mesoscale Model User's Workshop, Boulder, Colorado. October 28, 1993.

Bullock, O.R., Jr. 1993. A Workstation Concept for the Production of Dynamically-Constrained Meteorological Characterizations for Use in Air-Quality Modeling. Ninth International Conference on Interactive Information and Processing Systems for Meteorology, Oceanography, and Hydrology, Anaheim, California. January 17-22, 1993.

Bullock, O.R., Jr. 1991. The Effect of Sub-Grid-Scale Rainfall Analysis on Sulfate Wet Deposition Estimates in the Regional Lagrangian Model of Air Pollution (RELMAP). Seventh Joint Conference on Applications of Air Pollution Meteorology with AWMA, New Orleans, Louisiana. January 14-18, 1991.

Bullock, O.R., Jr. 1990. The Effects of Size-Dependent Dry-Deposition Velocities in an Eulerian Regional-Scale Particulate Model. Eighteenth NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Vancouver, British Columbia, Canada. May 13-17, 1990.

Ellen J. Cooter

(On assignment from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce).

Meteorologist
Atmospheric Modeling Division
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina
(919) 541-1334

Education

B.S., Meteorology, University of Oklahoma, 1976
M.S., Meteorology, University of Oklahoma, 1978
Ph.D., Meteorology, University of Oklahoma, 1985

Professional Experience

Meteorologist, NOAA Atmospheric Modeling Division, 1990-Present

Assistant State Climatologist, Oklahoma, 1981-1990
Graduate Research Assistant, University of Oklahoma, 1979-1981

North Dakota Weather Modification Board, Norman, Oklahoma, 1978-1979

Graduate Teaching Assistant, University of Oklahoma, 1977-1978

Professional Appointments and Memberships

American Association of State Climatologists, Associate Member, 1981-present
American Meteorological Society, Member, 1987-present
AMS Committee on Applied Climatology, 1991-present
Chair, AMS 9th Applied Climate Conference Program Committee, 1994-1995
Chair, AMS Committee on Applied Climatology, 1995-1997
Adjunct Assistant Professor of Agricultural Engineering, Oklahoma State University, 1986-1990
Editorial Advisor, Climate Research, 1990-present
Sigma Xi, Member, 1991-present
National Research Council Research Advisor, 1994-present
Adjunct Assistant Professor of Geography, North Carolina State University, Chapel Hill, 1992-present

Publications

Dhakhwa, G.B., C.L. Campbell, E.J. Cooter, and S.K. LeDuc. 1997. Use of Crop Models in Assessing the Interactive Effects of Global Warming and CO_2 Doubling on Maize Production. Agricul. Forest Meteorol., in press.

Sampson, D.A., E.J. Cooter, P.M. Dougherty, and H. Lee Allen. 1996. Comparison of the UKMO and GFDL GCM Climate Projections in NPP Simulations for Southern Loblolly Pine Stands. Climat. Res., 7(1): 55-69.

Cooter, E.J. and G.B. Dhakhwa. 1995. A Solar Radiation Model for Use in Biological Applications in the South and Southeastern USA. Agricul. Forest Meteorol., 78(1-2):31-51.

Cooter, E.J. and S.K. LeDuc. 1995. Recent Frost Date Trends in the North-Eastern USA. Internat. J. Climat., 15:65-75.

Cooter, E.J. and S.K. LeDuc. 1994. Recent Frost Date Trends in the Northeastern United States. In - Nathaniel Guttman (Ed.), NOAA National Environmental Watch (CD-ROM) Prototype-1994, National Climate Data Center, National Oceanic and Atmospheric Administration, Asheville, North Carolina..

Cooter, E.J., M.B. Richman, and P.J. Lamb. 1994. Documentation for the Southern Global Change Program Climate Change Scenarios. Report to the U.S. Forest Service, Southern Global Change Program Office, Raleigh, North Carolina, Interagency Agreement Number 29-1163.

Cooter, E.J., B.K. Eder, S.K. LeDuc, and L. Truppi. 1993. Climate Change Models and Forest Impact Research. J. Forest., 91(9):38-43.

Cooter, E.J., B.K. Eder, S.K. LeDuc, and L. Truppi. 1993. General Circulation Model Output for Forest Climate Change Research and Applications. U.S. Department of Agriculture, Forest Service, Southeastern Forest Experiment Station, Asheville, North Carolina. General Technical Report SE-85, 38 pp.

Brooks, R.T., T.S. Frieswyk, D.M. Griffith, E. Cooter, and L. Smith. 1992. New England's Forests: A Baseline for the New England Forest Health Monitoring Program. U.S. Department of Agriculture, Forest Service, Northeastern Forest Experiment Station, Radnor, Pennsylvania. Resource Bulletin NE-123, 89 pp.

Brooks, R.T., D.R. Dickson, W.G. Burkman, I. Millers, M. Miller-Weeks, E. Cooter, and L. Smith. 1992. Forest Health Monitoring in New England: 1990 Annual Report. U.S. Department of Agriculture, Forest Service, Northeastern Forest Experiment Station, Radnor, Pennsylvania. Resource Bulletin NE-125, 59 pp.

Cooter, E.J., S.K. LeDuc, and L. Truppi. 1992. Climate Research for Ecological Monitoring and Assessment: A New England example. Climat. Res., 2:101-112.

Cooter, E., and W. Cooter. 1991. Impacts of Greenhouse Warming on Water Temperature and Water Quality in the Southern United States. Climat. Res., 1(1):1-12.

Cooter, E.J., S.K. LeDuc, L. Truppi and D.R. Block. 1991. The Role of Climate in Forest Monitoring and Assessment: A New England Example. U.S. Environmental Protection Agency, Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, North Carolina. EPA-600/3-91-074, 109 pp.

Cooter, E. 1990. The Impact of Climate Change on Continuous Corn Production in the Southern U.S.A. Climat. Change, 16:53-82.

Cooter, E. 1990. A Heat Stress Climatology for Oklahoma. Phys. Geogr., 11(1):17-35.

Dr. M. Trevor Scholtz

Manager, Environmental Computing and Modelling and Director, Canadian Global Emissions Interpretation Centre
ORTECH Corporation
2395 Speakman Drive
Mississauga, Ontario, Canada L5K 1B3
(905) 822-4111, Ext. 524
Fax: (905) 823-1446
tscholtz@ortech.on.ca

Role in the Lake Michigan Mass Balance Project

Principal Investigator and project manager on a contract with ORTECH to supply hourly atrazine emissions data for the modelers in the LMMBS. The atrazine emissions will be computed using an air-surface exchange model driven by meteorological data supplied by the MM5 model.

Education

B.Sc., Chemical Engineering, University of Cape Town, 1958
M.A.Sc., Chemical Engineering, University of Toronto, 1961
Ph.D., Chemical Engineering, University of Toronto, 1965

Work Experience

Director of Research, TC Process Equipment, Scarborough, Ontario, Canada, 1965-1970

Senior Lecturer, Department of Chemical Engineering, University of Natal, South Africa, 1970-1978

Senior Consultant, Meteorological and Environmental Planning Company, Markham, Ontario, Canada, 1978-1984

Vice-President, Meteorological and Environmental Planning Company, Markham, Ontario, Canada, 1984-1989

Senior Scientist, ORTECH Corporation, Mississauga, Ontario, Canada, 1989-1994

Manager, Environmental Assessment Technologies and Director, Canadian Global Emissions Interpretation Centre, ORTECH Corporation, Mississauga, Ontario, Canada, 1994-1996

Manager, Environmental Computing and Modelling and Director, Canadian Global Emissions Interpretation Centre, Mississauga, Ontario, Canada, 1996-present

Experience

Preparation of regional and global emission inventories for criteria pollutants, metals and persistent organic pollutants.

Development of an emission data pre-processing system for preparing gridded emissions data for regional scale atmospheric transport, transformation and deposition models.

Processing of North American sulphur, nitrogen and volatile organic carbon emissions for input to the Canadian Regional Acid Deposition and Oxidants Model (ADOM).

Modeling of air movement and dispersion in a complex valley, and the development and evaluation of a supplementary control system.

Modeling and assessment of the dispersion from a gas turbine generating complex.

Modeling of dispersion from refinery complexes and acid plants.

Long-range transport modeling and assessment for major industrial sources.

Development of a meteorologically based emissions model for estimating emissions from open anthropogenic and natural sources.

Modeling of the transport, diffusion and volatilization of toxic organic substances from vegetated soils.

Modeling and assessment of dispersion with building wake and complex structure effects.

Preparation of meteorological, and geophysical driver fields for the Canadian Regional Acid Deposition and Oxidants Model (ADOM).

Development of a numerical planetary boundary layer model for the Canadian regional Acid Deposition and Oxidants Model (ADOM).

Modeling and assessment of moist plumes from cooling tower operation and environmental impact.

Real-time modeling of iceberg motion for operational applications.

Development of an operational ocean current model for predicting surface currents and current profiles on the Scotian Shelf.

Modeling of meteorologically forced ocean currents on the Scotian Shelf during the Canadian Atlantic Storms Project (CASP).

Publications

Scholtz, M.T., A.C. McMillan, C.F. Slama, Y-F. Li, N. Ting, and K.A. Davidson. 1997. Pesticide Emissions Modelling: Development of a North American Pesticide Emissions Inventory. Canadian Global Emissions Interpretation Centre Report CGEIC-1997-1.

Benkovitz, C.M., M.T. Scholtz, J. Pacyna, L. Tarrason, J. Dignon, E.C. Voldner, P.A. Spiro, J.A. Logan, and T.E. Graedel. 1996. Global Gridded Inventories of Anthropogenic Emissions of SO_2 and NO_x. J. Geophy. Res., 101(D22):39239-29253.

Li, Y-F., A.C. McMillan, and M.T. Scholtz. 1996. Global HCH Usage with 1° x 1° Latitude/Longitude Resolution. Environ. Sci. Technol., 30(12):3525-3533.

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Pacyna, J.M., M.T. Scholtz, and Y-F. Li. 1995. Global Budget of Metal Sources. Environ. Res., 3:145-159.

Scholtz, M.T., E.C. Voldner, and E. Pattey. 1994. Pesticide Volatilization Model Comparison with Field Measurements. In - Proceedings of the 87th AWMA Annual Meeting, Paper 94-MP5.03, 87(3A):1-12, Cincinnati, Ohio. June 19-24m, 1994.

Scholtz, M.T., C.F. Slama, and E.C. Voldner. 1993. Pesticide Emission Factors from Agricultural Soils. In - Proceedings of the 86th Annual AWMA Conference, Paper 93-MP-14.01, Denver, Colorado. June 13-18, 1993.

Scholtz, M.T. and E.C. Voldner. 1993. Modelling Air-Surface Exchange of Pesticides with Application to the Estimation of Emission. In - Proceedings of the First Workshop on Emissions and Modelling of Atmospheric Transport of Persistent Organic Pollutants and Heavy Metals, Durham, North Carolina, May 6-7, 1993. Sponsored by the U.S. Environmental Protection Agency and the Cooperative Program for Monitoring and Evaluation of the Long-Range Transmission of Air Pollutants in Europe., October 1993. Report Number EMEP/CCC 7/93-O-8917.

Scholtz, M.T. and E.C. Voldner. 1992. Estimation of Pesticide Emissions to the Air Resulting from Agricultural Applications. In - Proceedings of the 95th World Clean Air Congress and Exhibition, Volume 2, Paper IU-17B-01, Montreal, Quebec, Canada. August 30-September 4, 1992.

Scholtz, M.T., K.A. Davidson, and F. Vena. 1991. Preparation of a Canadian Inventory of Biogenic Volatile Organic Carbon Emissions from Vegetation. In - Proceedings of a Joint U.S. Environmental Protection Agency/AWMA Conference on Emission Inventory Issues in the 1990s, Durham, North Carolina. September 1991.

Scholtz, M.T., B. Weisman, L. Mahrt, and A.D. Christie. 1988. Generation of Meteorological Data Fields for the ADOM Eulerian Regional Model. In - Han van Dop (Ed.), Air Pollution Modelling and Its Application VI, Plenum Publishing Company, New York, New York.

Scholtz, M.T., D.G. McGillivray, B. Weisman, and D.A. Greenberg. 1987. Modelling of Meteorologically Forced Currents in the Scotian Shelf. In - Proceedings of Oceans '87 Conference, IEEE, Halifax, Canada, September 1987.

Scholtz, M.T., B. Weisman, A.D. Christie, and L. Mahrt. 1986. Generation of Meteorological Data Fields for the ADOM Eulerian Regional Model. American Meteorological Society, Proceedings of the Fifth Joint Conference on Applications of Air Pollution Meteorology with APCA, Chapel Hill, North Carolina. November 8-21, 1986.

Scholtz, M.T. and B. Weisman. 1985. A Multi-Layered, Long-Range, Transport, Lagrangian Trajectory Model: Comparison with Fully Mixed Single Layer Models. In - C. De Wispelaere (Ed.), Air Pollution Modelling and Its Application IV. Plenum Publishing Company, New York, New York.

Scholtz, M.T. and C.J. Brouchaert. 1978. Modelling of Stable Air Flows Over a Complex Region. J. Appl. Meteorol., 17:1249-1257.

Scholtz, M.T. and O. Trass. 1970. Mass Transfer in a Non-Uniform Impinging Jet, Part I: Stagnation Flow-Velocity and Pressure Distribution. AJChE J., 16:90-96.

Scholtz, M.T. and O. Trass. 1970. Mass Transfer in a Non-Uniform Impinging Jet, Part II: Stagnation Flow-Velocity and Pressure Distribution. AJChE J., 16:97-104.

Scholtz, M.T. and O. Trass. 1964. Mass Transfer in the Laminar Radial Wall Jet. AIChE J., 9:548.

Presentations

Scholtz, M.T. and E.C. Voldner. 1992. Air/Soil Exchange of Volatile Toxics. CIRAC/AWMA-OS Joint International Conference on Atmospheric Chemistry, Toronto, Ontario, Canada. January 1992.

Scholtz, M.T. and E.C. Voldner. 1989. Development of a Model for Predicting the Volatilization of Toxic Materials from Vegetated Soils. Tenth Annual Meeting of the Society of Environmental Toxicology and Chemistry, Toronto, Ontario, Canada. October 28-November 2, 1989.

Scholtz, M.T., K. Walsh, and L. Mahrt. 1986. A Study of Drought Onset Due to Interactions Between Soil Moisture and the Atmospheric Boundary Layer. Twentieth Annual Congress, Canadian Meteorological and Oceanographic Society, Regina, Canada. June 3-6, 1986.

Scholtz, M.T. and B. Weisman. 1980. A Model for Predicting Air Movement and Dispersion in a Complex Valley. 73rd Annual Meeting of the APCA, Montreal, Quebec, Canada. June 22-27, 1980.

Weisman, B. and M.T. Scholtz. 1980. Dispersion Model for Montreal East Development and Validation. 73rd Annual Meeting of the APCA, Montreal, Quebec, Canada. June 22-27, 1980.

David J. Schwab

Oceanographer
U.S. Department of Commerce
National Oceanic and Atmospheric Administration
Great Lakes Environmental Research Laboratory
2205 Commonwealth Boulevard
Ann Arbor, Michigan 48105
(734) 741-2120
Fax: (734) 741-2055
schwab@glerl.noaa.gov

Specializations and Research Interests

Fields of Specialization and Research Interests: Specialized in geophysical fluid dynamics problems in the Great Lakes and other shallow enclosed seas including theoretical, numerical, and observations investigations of circulation, thermal structure, seiches, storm surges, wind waves, and air-sea interaction. Current research interest - numerical modeling of three dimensional lake-scale circulation and thermal structure.

Education

Ph.D., Oceanic Science, University of Michigan, 1981
M.S., Physics, University of Wisconsin-Milwaukee, 1974
B.S. (Summa Cum Laude), Applied Mathematics and Physics, University of Wisconsin-Milwaukee, 1972

Professional Experience

Oceanographer, Great Lakes Environmental Research Laboratory, NOAA, 1980-present (GS-1360-13, 10/80; GS-1360-14, 8/84)

Physical Scientist, Great Lakes Environmental Research Laboratory, NOAA, 1975-1981 (GS-1301-11, 12/76; GS-1301-12, 10/78)

Adjunct Assistant Professor in Department of Geography, Atmospheric Sciences Program at the Ohio State University, 1992-present

Visiting Scientist, VAW/ETH - Zurich, Switzerland, 1982
Adjunct Assistant Professor in Atmospheric and Oceanic Science, Department of the University of Michigan, 1981-1982

Research Specialist, Center for Great Lakes Studies, University of Wisconsin-Milwaukee, 1975

Professional Honors and Awards

U.S. Department of Commerce, National Oceanic and Atmospheric Administration Outstanding Performance Award, 1979, 1980.
Selected outstanding graduate student in oceanography by the College of Engineering at the University of Michigan, 1981.
National Oceanic and Atmospheric Administration/Great Lakes Environmental Research Laboratory Distinguished Authorship Award, 1984.
U.S. Department of Commerce, National Oceanic and Atmospheric Administration Outstanding Performance Award, 1987, 1988, 1989, 1995, 1996.

Professional Affiliations

American Geophysical Union, American Meteorological Society, The Oceanography Society, International Association for Great Lakes Research (Treasurer, 1986-1989).

Review Panels Associate Editor, Journal of the Great Lakes Research. Journal of Geophysical Research Limnology and Oceanography, Journal of Physical Oceanography, American Society of Civil Engineers, Hydraulics Division, Canadian Journal of Water Pollution Research, Atmospheric-Oceanic Annales, Geophysicae, NOAA Sea Grant, International Joint Commission, National Science Foundation.

International Activities Workshop on Physical Limnology and Water Quality Modelling of Large Lake Systems, Petrozavodsk, Russia, October 19-23, 1992.

Contracts and Grants Awarded

Great Lakes CoastWatch Program, NOAA Coastal Ocean Program, 1990-92, $180K. Software Tools for CoastWatch.
NOAA Coastal Ocean Program, 1992, $10K Great Lakes Forecasting System (Co-Principal Investigator with K.W. Bedford).
NOAA Coastal Ocean Program, 1991-96, $750K, Coastal Hazards - Great Lakes Wind Forecasts.

NOAA Coastal Ocean Program, 1992-94, $150K, Lake St. Clair Macrophyte Study, Particle Trajectory Model for Lake St. Clair.
U.S. Army Corps of Engineers, 1995, $6K, Lake Michigan Mass Balance Study, Hydrodynamic Model of Lake Michigan.
U.S. Environmental Protection Agency, 1995-97, $336K.

Publications

Journals

Beletsky, D., W.P. O'Connor, D.J. Schwab, and D.E. Dietrich. 1997. Numerical Simulation of Internal Kelvin Waves and Coastal Upwelling Fronts. J. Phys. Oceanogr., in press.

Eadie, B.J., D.J. Schwab, G.A. Leshkevich, T.H. Johengen, R.A. Assel, N. Hawley, R.E. Holland, M.B. Lansing, P. Lavrentyev, G.S. Miller, N.R. Morehead, J.A. Robbins, and P.L. Van Hoof. 1996. Recurrent Coastal Plume in Southern Lake Michigan. EOS, Trans. Amer. Geophys. Union.,77(35):337-338.

Schwab, D.J. and K.W. Bedford. 1996. Great Lakes Forecasting, in Coastal Ocean Prediction. In - C. Moores (Ed.), American Geophysical Union Coastal and Estuarine Studies, in press.

Schwab, D.J. and D. Beletsky. 1996. Propagation of Kelvin Waves Along Irregular Coastlines in Finite-Difference Models. Submitted to Advances in Water Resources.

Schwab, D.J., W.P. O'Connor, and G.L. Mellor. 1995. On the Net Cyclonic Circulation in Large Stratified Lakes. J. Phys. Oceanogr., 25(6):1516-1520.

Schwab, D.J. and K.W. Bedford. 1994. Initial Implementation of the Great Lakes Forecasting System: A Real-Time System for Predicting Lake Circulation and Thermal Structure. Water Pollut. Res. J. Can., 29(2/3):203-220.

Leshkevich, G.A., D.J. Schwab, and G.C. Muhr. 1993. Satellite Environmental Monitoring of the Great Lakes: A Review of NOAA's Great Lakes CoastWatch Program. Photogram. Engin. Rem. Sens., 59(3):371-379.

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Schwab, D.J. 1992. A Review of Hydrodynamic Modeling in the Great Lakes From 1950-1990 and Prospects for the 1990's. In - F. Gobas and A. McQuorquodale (Eds.), Chemical Dynamics in Freshwater Ecosystems, pp., 41-62, Lewis Publishers, Incorporated, Chelsea, Michigan.

Schwab, D.J., G.A. Leshkevich, and G.C. Muhr. 1992. Satellite Measurements of Surface Water Temperature in the Great Lakes: Great Lakes CoastWatch. J. Great Lakes Res., 18(2):247-258.

Schwab, D.J., A.H. Clites, C.R. Murthy, J.E. Sandall, L.A. Meadows, and G.A. Meadows. 1989. The Effect of Wind on Transport and Circulation in Lake St. Clair. J. Geophys. Res., 94(C4):4947-4958.

Fahnenstiel, G.L., D. Scavia, G.A. Lang, J.H. Saylor, G.S. Miller, and D.J. Schwab. 1988. Impact of Inertial Period Waves on Fixed-Depth Primary Production Estimates. J. Plankton Res., 10:77-87.

Liu, P.C. and D.J. Schwab. 1987. A Comparison of Methods for Estimating U* from Given Uz and Air-Sea Temperature Differences. J. Geophys. Res., 92(C6):6488-6494.

Horn, W., C.H. Mortimer, and D.J. Schwab. 1986. Wind-Induced Internal Seiches in the Lake of Zurich, Observed and Modelled. Limnol. Oceanogr. 31(6):1232-1254.

Schwab, D.J. and J.R. Bennett. 1986. A Lagrangian Comparison of Objectively Analyzed and Dynamically Modeled Circulation Patterns in Lake Erie. J. Great Lakes Res., 13(4):515-529.

Schwab, D.J., J.R. Bennett, and E.W. Lynn. 1985. A Two-Dimensional Lake Wave Prediction System. Environ. Software, 1(1):4-9.

Liu, P.C., D.J. Schwab, and J.R. Bennett. 1984. Comparison of a Two-Dimensional Wave Prediction Model with Synoptic Measurements in Lake Michigan. J. Phys. Oceanogr., 14:1514-1518.

Schwab, D.J., J.R. Bennett, P.C. Liu, and M.A. Donelan. 1984. Application of a Simple Numerical Wave Prediction Model to Lake Erie. J. Geophys. Res., 89:3586-3592.

Schwab, D.J., G.A. Meadows, J.R. Bennett, H. Schultz, P.C. Liu, J.E. Campbell, and H. Dannelongue. 1984. The Response of the Coastal Boundary Layer to Wind and Waves: Analysis of an Experiment in Lake Erie. J. Geophys. Res., 89:8043-8053.

Schwab, D.J. and J.A. Morton. 1984. Estimation of Overlake Wind Speed from Overland Wind Speed: A Comparison of Three Methods. J. Great Lakes Res., 10:68-72.

Hutter, K., G. Salvade, and D.J. Schwab. 1983. On Internal Wave Dynamics in the Northern Basin of Lake of Lugano. Geophys. Astrophys. Fluid Dyn., 27:299-336.

Schwab, D.J. 1983. Numerical Simulation of Low-Frequency Current Fluctuations in Lake Michigan. J. Phys. Oceanogr., 13:2213-2224.

Schwab, D.J. and D.B. Rao. 1983. Barotropic Oscillations of the Mediterranean and Adriatic Seas. Tellus, 35A:417-427.

Schwab, D.J. 1982. An Inverse Method for Determining Wind Stress from Water Level Fluctuations. Dyn. Atmos. Oceans, 6:251-278.

Bennett, J.R. and D.J. Schwab. 1981. Calculation of the Rotational Normal Modes of Oceans and Lakes with General Orthogonal Coordinates. J. Comp. Phys., 44:359-376.

Rao, D.B. and D.J. Schwab. 1981. A Method of Objective Analysis for Currents in a Lake. J. Phys. Oceanogr., 11:739-750.

Schwab, D.J. 1981. Determination of Wind Stress from Water Level Fluctuations. Doctoral Dissertation in Oceanic Science at the University of Michigan, Ann Arbor, Michigan. 108 pp.

Schwab, D.J., R.A. Shuchman, and P.C. Liu. 1981. Wind Wave Directions Determined from Synthetic Aperture Radar Imagery and from a Tower in Lake Michigan. J. Geophys. Res., 86:2059-2064.

Schwab, D.J., P.C. Liu, H.K. Soo, R.D. Kistler, H.L. Booker, and J.D. Boyd. 1980. Wind and Wave Measurements Taken from a Tower in Lake Michigan. J. Great Lakes Res., 6:76-82.

Schwab, D.J. 1978. Simulation and Forecasting of Lake Erie Storm Surges. Mon. Wea. Rev., 106:1476-1487.

Schwab, D.J. 1977. Internal Free Oscillations in Lake Ontario. Limnol. Oceanogr., 22:700-708.

Schwab, D.J. and D.B. Rao. 1977. Gravitational Oscillations of Lake Huron, Saginaw Bay, Georgian Bay, and the North Channel. J. Geophys. Res., 82:2105-2116.

Mortimer, C.H., D.B. Rao, and D.J. Schwab. 1976. A Supplementary Note and Figure to "Free Surface Oscillations and Tides of Lakes Michigan and Superior" by C.H. Mortimer and E.J. Fee. Phil. Trans. Roy. Soc. London, Ser. A, 281:58-60.

Rao, D.B., C.H. Mortimer, and D.J. Schwab. 1976. Surface Normal Modes of Lake Michigan: Calculations Compared with Spectra of Observed Water Level Fluctuations. J. Phys. Oceanogr., 6:575-588.

Rao, D.B. and D.J. Schwab. 1976. Two-Dimensional Normal Modes in Arbitrary Enclosed Basins on a Rotating Earth: Application to Lakes Ontario and Superior. Phil. Trans. Roy. Soc. London, Ser. A, 281:63-96.

Reports and Other Publications

Beletsky, D. and D.J. Schwab. 1996. Hydrodynamic Modeling for the Lake Michigan Mass Balance Project. Proceedings, U.S. Environmental Protection Agency Workshop on Next Generation Environmental Models Computational Methods, in press.

Kelley, J.G.W., D.J. Welsh, D.J. Schwab, K.W. Bedford, B. Hoch, and J.S. Hobgood. 1996. High-Resolution, Short-Term Lake Forecasts for Lake Erie. In - M.L. Spaulding and R.T. Cheng (Eds.), Estuarine and Coastal Modeling, Proceedings of the Fourth International Conference, American Society of Civil Engineers, in press.

Schwab, D.J. and K.W. Bedford. 1996. GLCFS - A Coastal Forecasting System for the Great Lakes. Preprint AMS Conference on Coastal Oceanic and Atmospheric Prediction, American Meteorological Society, pp. 9-14.

Schwab, D.J., D. Beletsky, W.P. O'Connor, and D.E. Dietrich. 1996. Numerical Simulation of Internal Kelvin Waves with Z-Level and Sigma Level Models. In - M.L. Spaulding and R.T. Cheng (Eds.), Estuarine and Coastal Modeling, pp. 298-312. Proceedings of the Fourth International Conference, American Society of Civil Engineers.

Kaun, C.-F., K.W. Bedford, and D.J. Schwab. 1995. A Preliminary Analysis of the Lake Erie Portion of the Great Lakes Forecasting System for Springtime Heating Conditions. In - D. Lynch and A. Davies (Eds.), Quantitative Skill Assessments for Coastal Ocean Models, Volume 48, pp. 397-424. Coastal and Estuarine Studies, American Geophysical Union.

Schwab, D.J. and K.W. Bedford. 1995. Operational Three-Dimensional Circulation Modeling in the Great Lakes. Computer Modeling of Seas and Coastal Regions II., pp. 387-396. Computational Mechanics Publication, Boston, Massachusetts.

Schwab, D.J. and K.W. Bedford. 1995. Report of the First Annual Great Lakes Forecasting System (GLFS) User's Workshop. Ohio Sea Grant Program, Columbus, Ohio. 11 pp.

Schwab, D.J., K.W. Bedford, and F.H. Quinn. 1995. Overview of the Great Lakes Forecasting System. Preprint of the Eleventh International Conference on IIPS for Meteorology, Oceanography, and Hydrology, pp. 132-133. American Meteorological Society.

Bedford, K. And D. Schwab. 1994. The Great Lakes Forecasting System, An Overview. Proceedings of the 1994 National Conference on Hydraulic Engineering, pp. 197-201.

Kelley, J., C.-C. Yen, J. Hobgood, D. Schwab, and K. Bedford. 1994. Short-Term Forecasts for Lake Erie. Proceedings of the 1994 National Conference on Hydraulic Engineering, pp. 227-231.

Kelley, J., C.-C. Yen, K. Bedford, A.J. Hobgood, and D. Schwab. 1993. Coupled Lake Erie Air-Sea Storm Resolving Forecasts and Predictions, The Viento Project. Proceedings of the Third International Conference of Estuarine and Coastal Modeling, pp. 202-215. American Society of Civil Engineers, New York, New York.

O'Connor, W.P. and D.J. Schwab. 1993. Sensitivity of Great Lakes Forecasting System Nowcasts to Meteorological Fields and Model Parameters. Proceedings of the Third International Conference on Estuarine and Coastal Modeling, pp. 149-157. American Society of Civil Engineers, Waterway, Port, Coastal and Ocean Division.

Bedford, K. and D. Schwab. 1991. The Great Lakes Forecasting System - Lake Erie Nowcasts/Forecasts. Proceedings of the Marine Technology Society Annual Conference (MTS '91), pp. 260-264. Marine Technology Society, Washington, D.C.

Schwab, D.J., R.E. Jensen, and P.C. Liu. 1991. Comparative Performance of Spectral and Parametric Wave Prediction Models in Lake Michigan. Mechanics Computing in 1990's and Beyond, Volume 1 - pp. 363-367. Computational Mechanics, Fluid Mechanics, and Biomechanics, American Society of Civil Engineers, Columbus, Ohio.

Yen, C.-C., K. Bedford, and D. Schwab. 1991. Nowcast Protocol for the Great Lakes Forecasting System. In - M.L. Spaulding, *et al.* (Eds.), Proceedings of the Second International Conference of Estuarine and Coastal Modeling, pp. 140-148, Tampa, Florida, November 12-15, 1991. American Society of Civil Engineers, New York, New York.

Bedford, K.W. and D.J. Schwab. 1990. Preparation of Real-Time Great Lakes Forecasts. Cray Channels, Summer 1990, pp. 14-17.

Bedford, K.W., C-C. Yen, J. Kempf, D.J. Schwab, R. Marshall, and C. Kuan. 1990. A 3D-Stereo Graphics Interface for Operational Great Lakes Forecasts. Estuarine and Coastal Modeling Proceedings, pp. 248-257. WW Division/American Society of Civil Engineers, Newport, Rhode Island.

Bedford, K.W., C.J. Merry, and D.J. Schwab. 1989. Real-Time Lake Erie Current and Temperature Field Forecasting - An Integrated Modeling and AVHRR Methodology. ASPRS Technical Paper, Proceedings 1989 American Society of Photography and Remote Sensing, pp. 77-78.

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Schwab, D.J. 1988. A Numerical Wave Predictions Model for Personal Computers. Proceedings of the 21st International Conference on Coastal Engineering.

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Schwab, D.J. 1987. Great Lakes Wave Prediction Model. In - Great Lakes Forecasters Handbook, National Weather Service Training Seminar for Great Lakes Operational Marine Forecasting. 11 pp.

Schwab, D.J. and E.W. Lynn. 1987. Great Lakes Storm Surge Planning Program (SSPP). National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum ERL-GLERL-65, 9 pp.

Richardson, W.S., D.J. Schwab, Y.Y. Chao, and D.M. Wright. 1986. Lake Erie Wave Height Forecasts Generated by Empirical and Dynamical Methods - Comparison and Verification. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Ocean Products Center Technical Note, 23 pp.

Bennett, J.R., D.J. Schwab, and E.W. Lynn. 1985. "Pathfinder" - An Interactive Model for Trajectory Prediction in the Great Lakes. Proceedings of the First Conference on Applications of Real-Time Oceanographic Circulation Modeling, Sponsored by NOAA/NOS, Laurel, Maryland.

Schwab, D.J. and P.C. Liu. 1985. Intercomparison of Wave Measurements from a NOMAD Buoy and from a Waverider Buoy in Lake Erie. Proceedings MTS-IEEEC Conference Oceans '85. Ocean Engin. Environ., pp. 1131-1137.

Schwab, D.J., E.W. Lynn, and G.S. Spalding. 1985. User's Manual for GLERL Data Access System (GDAS). National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. GLERL Open File Report, 45 pp.

Schwab, D.J., J.R. Bennett, and E.W. Lynn. 1984. A Two-Dimensional Lake Wave Prediction System. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum ERL-GLERL-51, 70 pp.

Schwab, D.J., J.R. Bennett, and E.W. Lynn. 1984. "Pathfinder"-A Trajectory Prediction System for the Great Lakes. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum ERL-GLERL-53, 37 pp.

Bennett, J.R., A.H. Clites, and D.J. Schwab. 1983. A Two-Dimensional Lake Circulation Modelling System: Programs to Compute Particle Trajectories and the Motion of Dissolved Substances. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum ERL-GLERL-46, 51 pp.

Hutter, K. and D.J. Schwab. 1982. Baroclinic Channel Models. Versuchsanstalt fur Wasserbau, Hydrologie und Glaziologie, ETH-Zurich, Internal Report 162, 20 pp.

Schwab, D.J., J.R. Bennett, and A.T. Jessup. 1982. A Two-Dimensional Lake Circulation Modeling System. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum ERL-GLERL-38, 79 pp.

Schwab, D.J. and K. Hutter. 1982. Barotrophic and Baroclinic Eigenmodes of Lake of Zurich and Lake of Lugano. Versuchsanstalt fur Wasserbau, Hydrologie und Glaziologie, ETH-Zurich, Internal Report 164, 118 pp.

Schwab, D.J., P.C. Liu, J.R. Bennett, G.A. Meadows, H. Schultz, J.E. Campbell, and H. Dannelongue. 1982. Coastal Boundary Layer Study Records Response of Lake Erie to Storms. Coastal Oceanogr. Climat. News, 4:30-31.

Schwab, D.J., P.C. Liu, J.R. Bennett, and G.A. Meadows. 1981. Lake Erie Coastal Boundary Layer Study Measures Flux of Energy During Storms. Coastal Oceanogr. Climat. News, 4:10.

Schwab, D.J. and D.L. Sellers. 1980. Computerized Bathymetry and Shorelines of the Great Lakes. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Data Report ERL-GLERL-32, 21 pp.

Richardson, W.S. and D.J. Schwab. 1979. Comparison and Verification of Dynamical and Statistical Lake Erie Storm Surge Forecasts. National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan. NOAA Technical Memorandum NWS TDL-69, 19 pp.

Schwab, D.J. 1978. Storm Surge Studies on the Great Lakes. American Society of Civil Engineers Convention, Preprint 3353, 12 pp.

Schwab, D.J. 1978. Analytical and Empirical Response Functions for Storm Surges on Lake Erie. Proceedings of the International Symposium on Long Waves in the Ocean, Canadian Marine Sciences Directorate, Manuscript Report Series No. 53, pp. 140-144.

Schwab, D.J. 1977. An Objective Analysis Scheme for Lake Currents. International Field Year for the Great Lakes Bulletin No. 19, pp. 50-52.

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Presentations

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Dmitry Beletsky

Research Fellow
Cooperative Institute for Limnology and Ecosystem Research
The University of Michigan
National Oceanic and Atmospheric Administration
Great Lakes Environmental Research Laboratory
2205 Commonwealth Boulevard
Ann Arbor, Michigan 48105-2945
(734) 741-2360
Fax: (734) 741-2055
beletsky@glerl.noaa.gov

Role in the Lake Michigan Mass Balance Project

Numerical hydrodynamic modeling for the Lake Michigan Mass Balance Project with the Great Lakes version (Schwab and Bedford, 1994) of the Princeton Ocean Model of Blumber and Mellor (1987).

Education

Ph.D., Physical Limnology/Oceanography, Institute for Lake Research, Russian Academy of Sciences, St. Petersburg, Russia, 1992
M.S., Marine Engineering (Major in Oceanography), Russian Hydrometeorological Institute, St. Petersburg, Russia, 1982.

Professional Experience Related to Modeling

Consultant, Cooperative Institute for Limnology and Ecosystem Research, University of Michigan, 1994-1995

Visiting Scientist, National Oceanic and Atmospheric Administration, Great Lakes Environmental Research Laboratory, 1994-1995

Research Scientist, Institute for Lake Research, Russian Academy of Science, St. Petersburg, 1992-1994

Assistant Research Scientist, Institute for Lake Research, Russian Academy of Science, St. Petersburg, 1989-1992

Research Assistant, Institute for Lake Research, Russian Academy of Science, St. Petersburg, 1986-1989

Research and Teaching Assistant, Russian Hydrometeorological Institute, St. Petersburg, 1985-1986

Projects Related to Modeling

Lake Circulation Model Studies, 1994-1995
Hydrodynamic Modeling of Lake Ladoga, 1992-1994
Hydrodynamic Modeling of Lake Onega, 1986-1992
Hydrodynamic Modeling of the White Sea, 1985-1986

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Dale J. Patterson

Chief, Water Quality Modeling Section
Wisconsin Department of Natural Resources
WT/2, Box 7921
Madison, Wisconsin 53707
(608) 266-0155
Fax: (608) 267-2800
patted@dnr.state.wi.us

Role in the Lake Michigan Mass Balance Project

I have been involved in the Mass Balance Modeling project beginning with the Green Bay/Fox River Mass Balance. In that project, I designed the sampling program for all water column, sediment, point source and runoff samples taken upstream of the DePere dam. I also designed the sampling program for sediments and point sources below the DePere dam. I supervised the application of the WASP4 model to the river upstream of the DePere dam and served on the Modeling Committee.

For the Lake Michigan Mass Balance, I have participated on the Modeling Committee, but have not been directly involved in data collection or modeling. I anticipate being involved in modeling of tributary loads at key sites to provide estimates of contaminant loadings to supplement direct load calculations being done with collected tributary data.

Education

B.S., Applied Mathematics and Physics, University of Wisconsin, 1970
M.S., Civil and Environmental Engineering, University of Wisconsin, 1981

Experience Related to Mathematical Modeling

I have worked with the Wisconsin Department of Natural Resources since 1973 as a water quality modeler. I have developed wasteload allocations for several segments of significant rivers in the state. These segments had multiple dischargers that were overloading the streams and required reductions below the levels of categorical effluent limits to correct dissolved oxygen problems due to excessive organic loads. These model required development of special techniques to determine the oxygen demand of paper and pulp mill waste. Conventional methods were not adequate for this task. Prior to the development of this long term BOD method, dissolved oxygen models were not successfully predictive.

Since 1987, I have been involved with development of PCB and sediment transport models on the Fox and other rivers in Wisconsin. This work included design and collection of PCB and related data for 40 miles of the Fox River where PCBs are known to be present in significant quantities. Delineation of sediment deposits and measurement of the concentration and mass of PCB present were primary aims to provide data to drive transport models. Water column collection provided data to calibrate and verify the models predictive capability.

Publications

Polychlorinated Biphenyl (PCB) Contaminated Sediment in the Lower Fox River: Modeling Analysis of Selective Sediment Remediation. Wisconsin Department of Natural Resources, Madison, Wisconsin. Publication WT-482-97, 1997.

Steuer, J., S. Jaeger, and D. Patterson. 1995. A Deterministic PCB Transport Model for the Lower Fox River Between Lake Winnebago and DePere, Wisconsin. Wisconsin Department of Natural Resources, Madison, Wisconsin. Publication WR 389-95, 283 pp.

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Wisconsin Department of Natural Resources. 1973. Water Quality Modeling of the Fox River. Wisconsin Department of Natural Resources, Madison, Wisconsin.

Mark Velleux, P.E.

Water Resources Engineer
Wisconsin Department of Natural Resources
P.O. Box 7921
Madison, Wisconsin 53707-7921
(608) 267-5262
Fax: (608) 267-2800
vellem@dnr.state.wi.us

Role in the Lake Michigan Mass Balance Project

Develop contaminant transport models for major Lake Michigan tributaries: Fox, Sheboygan, and Milwaukee Rivers. Model results used to estimate tributary loads for Level 2 to Lake Michigan mass balance model. Contribute to development of the IPX framework for tributary and lake models.

Education

M.S., Civil and Environmental Engineering, Clarkson University, 1993
B.S., Civil and Environmental Engineering, University of Michigan, 1987

Training

Modeling Fate and Transport of Toxic Substances in Surface and Ground Waters, 33rd Seminar Institute in Water Quality Control, Manhattan College, New York, June 1988.
Storm Water Management Modeling Workshop (SWMM 4.2), U.S. Environmental Protection Agency, Detroit, Michigan, September 1992.

Experience

Water Resource Engineer, Wisconsin Department of Natural Resources, 1994-Present. Develop couple sediment and contaminant transport models for Great Lakes tributaries; estimate contaminant export from tributaries to receiving waterbodies. Responsible for development of PCBV transport model for the Fox River downstream of DePere. Responsible for the continued development of the IPX water quality modeling framework.

Senior Mathematical Modeler, AScI Corporation, USEPA, LLRS, Grosse Ile, Michigan, 1991-1994. Developed coupled sediment and contaminant transport models for Great Lakes tributaries. Contributed to the Green Bay Mass Balance Study. Responsible for continued development of contaminant transport models for the Fox River and initial development of the IPX water quality modeling framework.

Research Assistant, Clarkson University/University of Buffalo, Potsdam/Buffalo, New York, 1990-1991. Developed couple sediment and contaminant transport for PCBs in the Fox River, Wisconsin and mirex in the Oswego River, New York. Contributed to the GBMBS.

Mathematical Modeler, AScI Corporation, USEPA, LLRS, Grosse Ile, Michigan, 1988- 1990. Developed a far-field contaminant transport model for PCBs in Saginaw Bay, Michigan, to examine the impact of contaminant migration from confined disposal facilities. Contributed to the GBMBS. Responsible for initial development of the PCB transport and fate model for the Fox River downstream of DePere.

Publications

Velleux, M., J. Gailani, and D. Endicott. 1996. Screening-Level Approach for Estimating Contaminant Export from Tributaries. J. Environ. Engin., 122(6):503-514.

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Presentations

Velleux, M.L., D. Endicott, and K. Freeman. 1993. A Mass Balance Model for Estimating Contaminant Export from the Lower Fox River to Green Bay. 36th Conference on Great Lakes Research, International Association for Great Lakes Research, St. Norbert College, DePere, Wisconsin. June 4-10, 1993.

Velleux, M.L., D. Endicott, and J. DePinto. 1991. A Mass Balance Analysis of Contaminant Transport and Fate in the Lower Fox River. 34th Conference on Great Lakes Research, International Association for Great Lakes Research, State University of New York at Buffalo, Buffalo, New York. June 3-6, 1991.

Martin, J.L., M. Velleux, and K. Rygwelski. 1989. Screening Level PCB of Model of Green Bay, Lake Michigan. 32nd Conference on Great Lakes Research, International Association for Great Lakes Research, University of Wisconsin, Madison, Wisconsin. May 30-June 2, 1989.

Velleux, M.L., J. Martin, J. Rathbun, and R. Kreis, Jr. 1989. Predicted and Observed Impacts of Contaminant Transport from the Saginaw Bay Diked Facility. Tenth Annual Meeting of the Society of Environmental Toxicology and Chemistry, Toronto, Ontario, Canada. October 28-November 2, 1989.

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Thomas M. Cole

Research Hydrologist
U.S. Army Engineer Waterways Experiment Station
CEWES-ES-Q
3909 Halls Ferry Road
Vicksburg, Mississippi 39180-6199
(601) 634-3283
Fax: (601) 634-3129
tcole@lasher.wes.army.mil

Role in the Lake Michigan Mass Balance Project

Implement the QUICKEST/ULTIMATE higher-order transport scheme into the IPX water quality model and link the POM to IPX.

Education

B.S., Aquatic Biology/Chemistry, Southwest Texas State University, 1978
M.S., Biology/Computer Science, Southwest Texas State University, 1982
Completed coursework for Ph.D., Environmental Engineering/Mathematics, Texas Technological University, 1987
Completed coursework for Ph.D., Environmental Engineering, Portland State University, 1996

Training

Lake and Reservoir Water Quality Modeling, Duke University, one week 1987
Cray Supercomputer Training, one week, 1988
Modeling of Transport, Fate, and Bioaccumulation of Toxic Substances in Surface Water, Manhattan College, one week, 1994

Awards

Meritorious Civilian Service Award, 1991
Commander and Director's Research and Development Achievement Award, WES, 1991
Outstanding Planning Achievement Award, Baltimore District, 1991
Outstanding Planning Achievement Award, North Atlantic Division, 1991
Department of the Army Research and Development Award, 1992
Technology Transfer Award, USEPA, 1995
Wesley H. Homer Award, American Society of Civil Engineers, Journal of the Environmental Engineering, 1995.

Publications

Cole, T.M. 1997. Application of CE-QUAL-W2 to J. Strom Thurmond Reservoir. To be published as WES TR. Draft submitted to sponsor and returned for revisions. Publication in 1997.

Tillman, D.H., T.M. Cole, and B. Bunch. 1997. Detailed Reservoir Water Quality Modeling (CE-QUAL-W2), Alabama-Coosa-Tallapoosa/ Apalachicola-Chattahoochee-Flint (ACT/ACF) Comprehensive Water Resource Study. To be published as WES TR. Draft submitted to sponsor, returned for revisions, and revisions complete. Publication in 1997.

Li, S.G., T. Cole, F. Ruan, and D.B. McLaughlin. 1996. A Generalized Analytical Testing Technique for Hydrologic Models. In - Proceedings of International Conference on Computational Methods in Water Resources, pp. 19-26, Cancun, Mexico. July 22-26, 1996.

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Harberg, M., D. Latka, T. Cole, J. Nestler, and G. Ploskey. 1994. Development of Fisheries Models for the Missouri River System. In - Proceedings of the 21st Annual Conference of the Water Resources Planning and Management Division, American Society of Civil Engineers, Denver, Colorado.

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Chapman, R. S. and T.M. Cole. 1992. Improved Thermal Predictions in CE-QUAL-W2. Proceedings of Water Forum '92, American Society of Civil Engineers, Baltimore, Maryland, August 1992.

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Cole, T.M. and H.H. Hannan. 1990. Dissolved Oxygen Dynamics. In - Thornton, Kimmel, and Payne (Eds.), Reservoir Limnology - Ecological Perspectives, Chapter 3, John Wiley and Sons, Incorporated, New York, New York.

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Cole, T.M. and H.H. Hannan. 1981. Application of the LARM Computer Model to Canyon Reservoir. Report to the U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi. Contract DACW39-81-M-0822.

Hannan, H.H. and T.M. Cole. 1979. Water Quality Analysis of Canyon Reservoir Data. Report to the U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, Mississippi. Contract DACW39-79-M-2987.

Mark S. Dortch

Supervisory Research Civil Engineer, GS-15
Chief, Water Quality and Contaminant Modeling Branch
Environmental Processes and Effects Division
Environmental Laboratory
U.S. Army Corps of Engineers
Waterways Experiment Station
ES-Q
3909 Halls Ferry Road
Vicksburg, Mississippi 39180-6199
(601) 634-3517
Fax: (601) 634-3129
dortchm@ex1.wes.army.mil

Education

B.S., Aerospace Engineering, Mississippi State University, 1971
M.S., Engineering, Mississippi State University, 1972
Ph.D., Civil Engineering, Colorado State University, 1990

Expertise

Water quality and contaminant modeling of surface water
Transport processes and numerical modeling of transport
Linkage of hydrodynamic and water quality models
Groundwater contaminant transport modeling
Wetland water quality treatment

Professional Expertise

Research Hydraulic Engineer, WES Hydraulics Laboratory, 1972-1983. Physical model studies of hydraulic structures; studies of reservoir hydrodynamics, stratified flow, and mixing; and numerical reservoir thermal modeling studies.

Chief, Water Quality and Contaminant Modeling Branch, WES Environmental Laboratory, 1983-Present. Water quality and contaminant modeling of all types of surface water systems; lead the development of simulators for subsurface in-situ contaminant remediation.

Professional Activities and Awards

Member of ASCE (Fellow Grade), AGU, and Sigma Xi
Associate Editor of ASCE Journal of Hydraulic Engineering, 1990-1994
Produced 90 technical publications
Registered Professional Engineer in Mississippi
Herbert D. Vogel WES Engineer Award, 1991
North Atlantic Division, USACE, Outstanding Planning Achievement Award, 1991
Department of Army Meritorious Civilian Service Award, 1991
Commanders Research and Development Achievement Award, 1991
Department of Army Research and Development Achievement Award, 1992

Training

Technical Report Writing (OPM, three days, 1973)
Water Quality Modeling for Rivers and Reservoirs (HEC, one week, 1976)
Mathematical Modeling of Environmental Systems (Manhattan College, one week, 1974)
Value Engineering (OPM, two days, 1975)
Radiological Monitoring (OPM, two days, 1978)
Statistical Hydrology (Colorado State University, one week, 1978)
Technical Writing (Shipley Associates, three days, 1981)
Supervision and Group Performance (three days, 1983)
Dale Carnegie Course (WES-EL through contractor, five days, 1985)
Workshop for First Line Managers (Mississippi Research and Development Center, three days, 1985)
Several computer short courses (WES, one to two days each, 1970s-1980s)
Lake and Reservoir Water Quality Modeling (Duke University, one week, 1987)
WES Management Seminar (WES through contractor, two days, 1987)
Modeling Fate of Toxic Substances (University of Colorado, three days, 1988)
Oil Spill Modeling (San Diego, California, three days, 1991)
Groundwater Contaminant Transport Modeling (University of Vermont, three days, 1991)
MINTEQA2 Metals Speciation Equilibrium Modeling (WES by USEPA, three days, 1991)

Groundwater Flow and Transport Modeling (University of Colorado, one week, 1991)
Multiphase Flow and Transport Modeling in Porous Media (WES, three days, 1991)
Hazardous/Radioactive Waste Management, WERC Videoconference Training Series (four 4-hour satellite video series, 1991)
World Oil Spill Model (WOSM) training course (ASA, Inc., three days, Narragansett, Rhode Island, 1992 and 1993)
Labor Relations Short Course (WES, three days, 1992)
Developmental Assignment (CERD-C, Washington, D.C., four months, 1993)
Executive Development Seminar (Arlington, Virginia, four days, 1995)
Leadership Development Program, Conducted by Center for Creative Leadership (San Diego, California, six days, 1996)
CE Executive Development Program (graduated November 1996)
Introduction to Neural Networks (WES, three days, 1996)
Introduction to HPC Parallel Processing (WES, one day, 1996)

Role in the Lake Michigan Mass Balance Project

Serve as WES oversight for work being conducted with Mr. Thomas Cole and Dr. Ray Chapman.

Publications

Li, Y., A.J. Mehta, K. Hatfield, and M.S. Dortch. 1997. Modulation of Constituent Release Across the Mud-Water Interface by Water Waves. Water Res. Res., 33(6):1409-1418.

Hall, R.W. and M.S. Dortch. 1995. New Jersey Nearshore Hypoxia during the Summer 1976. Proceedings of the Fourth International Conference on Estuarine and Coastal Modeling, San Diego, California. October 26-18, 1995.

Dortch, M.S. and C.F. Cerco. 1993. Chesapeake Bay Water Quality Model. In - Tom Patin (Ed.), Management of Bottom Sediments Containing Toxic Substances, Proceedings of the 16th U.S.-Japan Experts Meeting on Management of Contaminated Sediments, October 1993, Kitakyushu, Japan.

Dortch, M.S., R.S. Chapman, and S.R. Abt. 1992. Application of Three-Dimensional, Lagrangian Residual Transport. J. Hydr. Engin., 118(6):831-848.

Dortch, M.S. and B.H. Johnson. 1992. Hydrodynamics for Water Quality Models. In - Marshall Jennings and Nani Bhowmilk (Eds.), Hydraulic Engineering: Saving a Threatened Resource - In Search of Solutions, Proceedings of Water Forum 92, pp. 145-150. American Society of Civil Engineers, Baltimore, Maryland, August 1992.

Dortch, Mark S. 1991. Long-Term Water Quality Transport Simulations for Chesapeake Bay. In - J.H.W. Lee and Y.K. Cheung (Eds.), Proceedings of the International Symposium on Environmental Hydraulics, pp. 765-769, University of Hong Kong, Hong Kong, December 16-18, 1991. A.A. Balkema Publishers, Rotterdam.

Dortch, M.S. 1990. Three-Dimensional, Lagrangian Residual Transport Computed from an Intratidal Hydrodynamic Model. Doctoral Dissertation, Department of Civil Engineering, Colorado State University, Fort Collins, Colorado.

Dortch, M.S., R.S. Chapman, J.M. Hamrick, and T.K. Gerald. 1989. Interfacing 3-D Hydrodynamic and Water Quality Models of Chesapeake Bay. In - Malcolm Spaulding (Ed.), Proceedings of Conference on Estuarine and Coastal Modeling, pp. 182-191. American Society of Civil Engineers, Newport, Rhode Island, November 1989.

Dortch, Mark S. 1988. Approach for 3-D, Time-Varying Hydrodynamic and Water Quality Model of Chesapeake Bay. In - Steven R. Abt and Johannes Gessler (Eds.), Hydraulic Engineering, Proceedings of the 1988 National Conference, pp. 920-925. Hydraulic Division, American Society of Civil Engineers, Colorado Springs, Colorado, August 8-12, 1988.

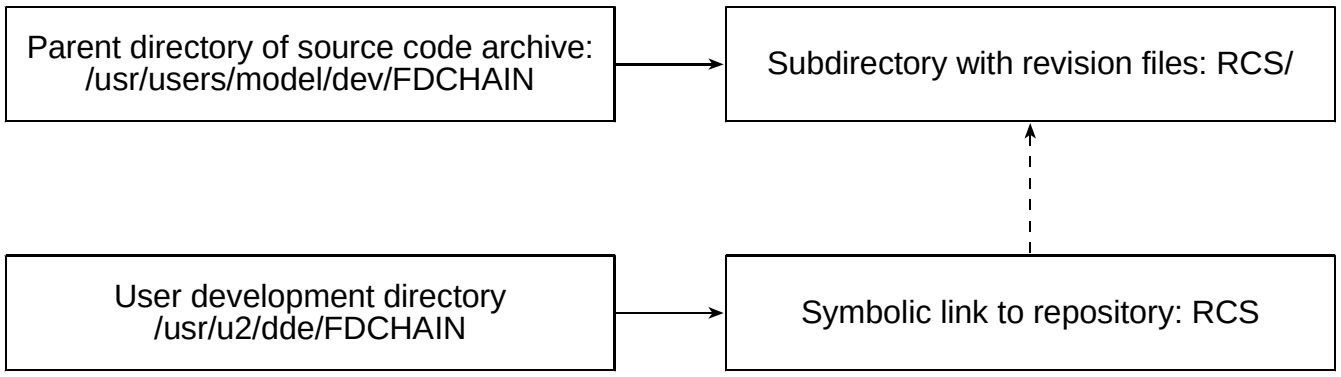
Appendix C
Revision Control System

Introduction

The following is a brief overview of the UNIX commands needed for using the Revision Control System or RCS code management. Several example commands are provided below. However, this document is not intended as a comprehensive manual of RCS. More detailed discussions of RCS and source code revision control in general can be found elsewhere. (See, for instance, Daniel Gilly's discussion of RCS and SCCS in UNIX in a Nutshell: System V Edition - Oreilly, 2nd Edition, June 1992.)

Unix Directories

By convention, each application, i.e., each model or utility program, as a directory associated with it. The relationship between the user's development directory and the RCS repository for the respective application is shown in the figure below. The UNIX command for creating a symbolic link to the repository directory is shown in the figure.



LLRS Implementation: File Names

The following conventions are being followed for application source files:

- FORTRAN Modules - i.e., subroutines and functions - are each given separate files. File names corresponding to FORTRAN modules are given the suffix .F (earlier versions of FDCHAIN, IPX, and UT were given the file suffix .FORTRAN. Please refer to http://hobbes.grl.epa.gov/MODELING/dev.html for a discussion of the development of these applications (internal to LLRS, will be available on internet when MED-Duluth, Web Page is established in the future). FORTRAN include files containing parameter definitions and common blocks are given the file suffix .inc, while cpp header file names are given the suffix .h.

- All standard C function file names are given the suffix .c. C include files are given the standard file suffix .h.

- Repository s-files - i.e., those contained in the subdirectory RCS have the additional file suffix,.v appended to their names.

The Cheat Sheet

rlog Commands

The following commands are used to show revision information:

RCS Command	Explanation
rlog RCS/*	Show detailed revision information for all source files
rlog -R RCS/*	Show a all revision files
rlog RCS/filename	Show revision information for source file filename
rlog filename	Show revision information for source file filename
rlog -r1.1.1 filename	Show revision information for branch 1.1.1 of filename
rlog -R -L RCS/*	Show revision information for all files that do not have locks set
rlog _R _L -lusername RCS/*	Show files locked by the user username
rlog -d01-June-1996/<31-December-1996 filename	Show all revisions made to filename between 1-June-1996 and 31-December-1996. Note the backslash

co Commands

The following commands are used to check out or retrieve files from the RCS repository:

RCS Command	Explanation
co filename	Check out source file filename from the default branch
co -q filename	Check out source file filename quietly (no diagnostics) from the default revision branch
co -r1.1.1 filename	Check out the latest revision of filename from branch 1.1.1
Co -I1.1.1 filename	Check out and lock the latest revision of filename from branch 1.1.1
Co -u1.1.1 filename	Check out and unlock the latest revision of filename from branch 1.1.1. Note: you must already have a lock on the corresponding revision

ci Commands

The following commands are used to check in files to the RCS repository. All of these commands assume that the revision corresponding to the modified file has already been locked by the user.

RCS Command	Explanation
ci filename	Check in source file filename
ci -q filename	Check in source file filename quietly (no diagnostics)
ci -r1.1.1 filename	Check in source file to the revision branch 1.1.1. This is usually not necessary.
Ci -f filename	Force the check in of a source file filename. Check in is not normally done if no modifications were made.
Ci -1 filename	Check in the source file filename, then check out and lock again
ci -u filename	Check in the source file filename, then check out (unlocked) again

rcsdiff Commands

Because the RCS s-files contain both the source and its revision information, direct comparison of a revised source file with an RCS s-file is impractical. The RCS command rcsdiff allows the user to compare a checked out version of a file with any previous revision of that file, for the purpose of identifying recent modifications to the source.

RCS Command	Explanation
rcsdiff filename	Show differences between the user file filename and its most recent revision in the default branch
rcsdiff -r1.1.1 filename	Show differences between the user file filename and the last revision in the branch 1.1.1
Rcsdiff -r1.1.1.3 filename	Show differences between the user file filename and the specific revision 1.1.1.3
Rcsdiff -r1.1.1.3 -r1.1.1.4 filename	Show differences between revisions 1.1.1.3 and 1.1.1.4 of the source file filename

An Example Session

In the example below, the user makes modifications to a source file for the FDCHAIN application. The symbolic link to the FDCHAIN RCS repository only needs to be made if it is not already present. The user reviews the revision information for a specific file, and checks out two files. The user intends to modify the files being checked out, and locks them at check out time. Only one file is modified, but the user desires that both files be checked in as new revisions. The modified file can be checked in normally; however, the unmodified file must be checked in using the -f flag, otherwise no new revisions will be registered by the source code management. The user than reviews the revision information for the two files.

```
% cd                          # Go to home directory.
% cd FDCHAIN development      # Go to FDCHAIN directory
% ln -s ~model/dev/FDCHAIN/RCS  # Make symbolic link to repository
% flog bioengi.F              # See revisions for a file
% co -16.0.1 bioeng1.F        # Check out and lock first file
% co -16.0.1 bioeng2.F        # Check out and lock second file
% vi bioeng1.f                # Edit the file
% rcsdiff bioeng1.F           # Compare with last checked in revision
% ci bioeng1.F                # Check in first file
% ci -f bioeng2.F             # Force check in of second file
% rlog bioeng1.F bioeng2.F    # See revision information of both files
```

Conclusion

A brief review of the RCS directory structure and commands has been provided. Example commands for examining revision information, retrieving and checking in source, and examining differences between source revisions has been provided. Review of the RCS administrator's command rcs has been intentionally avoided as that utility and its functions are not generally pertinent to the users' interaction with the source code management system.

Appendix D
Project Approvals

Branch/Team/Project Management Approvals

William L. Richardson
LMMBP Modeling Workgroup Chair _____ *Signature* *Date*

Douglas D. Endicott
CBSSS Team Leader _____ *Signature* *Date*

Russell G. Kreis, Jr.
CBSSS Chief _____ *Signature* *Date*

Health and Safety Approvals

Eric S. Mead
SHEMP Manager **NOT APPLICABLE** *Signature* *Date*

Eric S. Mead
Radiation Safety Officer **NOT APPLICABLE** *Signature* *Date*

Eric S. Mead
Chemical Assessment Committee Chair **NOT APPLICABLE** *Signature* *Date*

Quality Assurance Approvals

Allan R. Batterman
QA Manager _____ *Signature* *Date*

Jose A. Serrano
Quality of Science Committee Chair _____ *Signature* *Date*

Animal Care and Use Approvals

Virginia Snarski **NOT APPLICABLE**
Animal Care and Use Committee Chair _____ *Signature* *Date*

Senior Management Approvals

Vacant
Acting Associate Director of Science _____ *Signature* *Date*

Steven P. Bradbury
Acting Division Director _____ *Signature* *Date*

Note: When all above signatures are obtained the QAPP has been completely reviewed and approved.

Project QAPP Concurrence

Louis Blume
QA Manager, GLNPO _____ *Signature* *Date*

Great Lakes National Program Office Approval

Paul Horvatin
Division Director _____ *Signature* *Date*

Subproject Approvals

The following signatures signify that their portions of this document are current and accurate to the best of their knowledge.

Victor J. Bierman, Jr. Limno-Tech, Inc.	*Signature*	*Date*
Ellen Cooter USEPA-AMD, RTP	*Signature*	*Date*
Thomas Cole USACOE-WES	*Signature*	*Date*
Robert Day MDEQ	*Signature*	*Date*
Gerald Keeler University of Michigan	*Signature*	*Date*
Keri Hornbuckle SUNY at Buffalo	*Signature*	*Date*
Mark Velleux WDNR	*Signature*	*Date*
David Schwab NOAA-GLERL	*Signature*	*Date*

Appendix E
Model Development and Progress

As stated in the main report, many of the sub-models are being developed as part of the project. They are all at different stages of development which is difficult to communicate in a report that has taken months to prepare and finalize. By the time this report is published, the models will have progressed even further. To communicate to managers, participants, and reviewers the progress of this work, modelers are now being asked to maintain a status sheet indicating the various model levels and stages of their work. Those wishing to receive this report should make their request by sending an E-mail message to Bill Richardson: wlr@lloyd.grl.epa.gov or call (734) 692-7611.

Appendix F
Lake Michigan Mass Balance Project Committees, Workgroups, and Personnel
(At the time QAPP was Approved - November 1994 Through February 1995)

Executive Steering Committee:

Barry DeGraaf, Acting Director, Water Division, USEPA, Region 5, Chicago, Illinois

Lloyd Eagan, Air Division, WDNR, Madison, Wisconsin

Christopher Grundler, Director, USEPA, GLNPO, Chicago, Illinois

Steven Hedtke, Director, USEPA, MED-Duluth, Duluth, Minnesota

Melissa McCullough, USEPA, Office of Air Quality Planning and Standards, Washington, D.C.

Richard Powers, Assistant Chief, Michigan Department of Natural Resources, Surface Water Quality Division, Lansing, Michigan

QA Program Plan Cooperators:

Daniel Bauer, USGS, Water Resources Division, Middleton, Wisconsin

Brian Eadie, NOAA, GLERL, Ann Arbor, Michigan

John Gannon, USGS, National Biological Survey, Ann Arbor, Michigan

Paul Horvatin, USEPA, GLNPO, Chicago, Illinois

Technical Coordinating Committee:

Paul Horvatin, Co-Coordinator, USEPA, GLNPO, Chicago, Illinois

Brian Eadie, Sediment Co-chairperson, NOAA, GLERL, Ann Arbor, Michigan

Robert Day, Chairperson, Tributary Load Committee, Michigan Department of Natural Resources, Lansing, Michigan

William Richardson, Chairperson, Modeling Workgroup, USEPA, CBSSS, LLRS, Grosse Ile, Michigan

John Gannon, Biota Co-chairperson, USGS, NBS, Ann Arbor, Michigan

Louis Blume, Chairperson, QA and Data Coordinator, USEPA, GLNPO, Chicago, Illinois

Appendix G
Quality Systems and Implementation Plan (QSIP)

Project Title

Estimation of Contaminant Loading From Monitored and Unmonitored Tributaries to Lake Michigan for the USEPA Lake Michigan Mass Balance Study.

Principle Investigator

David Hall, USGS, 8505 Research Way, Middleton, Wisconsin 53562 (608) 821-3875.

EPA Project Officer

Mr. Glenn Warren, USEPA, GLNPO, 77 West Jackson, Chicago, Illinois 60604-3590.

Submitted

October 23, 1998.

Project Planning and Organization

Introduction

The USEPA requires that all environmental projects mandated or funded by the USEPA develop a reviewed and approved quality assurance (QA) program as summarized in a written QA Project Plan (QAPP). The purpose of the QAPP is to demonstrate that: intended measurements are appropriate for achieving project objectives; quality control procedures are sufficient for obtaining data of known and adequate quality; and such data will be defensible if challenged technically or legally (USEPA, 1991). A Quality Systems and Implementation Plan (QSIP) may be used to describe specific aspects of a project as a supplement to the project QAPP. This QSIP describes methods used to compute loads for both monitored and unmonitored tributaries to Lake Michigan in support of the USEPA LMMBP.

Background

Annex 2 of the 1972 GLWQA (amended in 1978, 1983, and 1987) between the United States and Canada called for development of LaMPs for each of the Great Lakes. The LaMPs document approaches to reduce inputs of toxic chemicals and other pollutants to each Great Lake. The LMMBP was developed in 1993 as part of the LaMP for Lake Michigan. The primary objective of the LMMBP was to provide an information base from which to guide federal, state, and local toxic load reduction efforts in the Lake Michigan basin (USEPA, 1997). An overview of the LMMBP has been published in the Lake Michigan Mass Budget/Mass Balance Workplan (USEPA, 1995). Additional information describing the LMMBP can be found on the USEPA Mass Balance Internet homepage at "http://www.epa.gov/grlakes/lmmb".

The Lake Michigan Tributary Project (LMTMP) is a sub-project of the LMMBP. The overall objective of the LMTMP is to obtain estimates of contaminant loading to Lake Michigan from all tributaries, both monitored and unmonitored. The LMTMP was supported by the USEPA and was conducted as a cooperative effort between the USGS, the Wisconsin Department of Environmental Quality, the Michigan Department of Environmental Quality, the Wisconsin State Laboratory of Hygiene, the University of Wisconsin Water Chemistry Program, and Rutgers University.

As part of the LMTMP, eleven major tributaries to Lake Michigan (Figure 1, Table 1) were sampled from April 1994 through October 1995. Tributaries monitored were

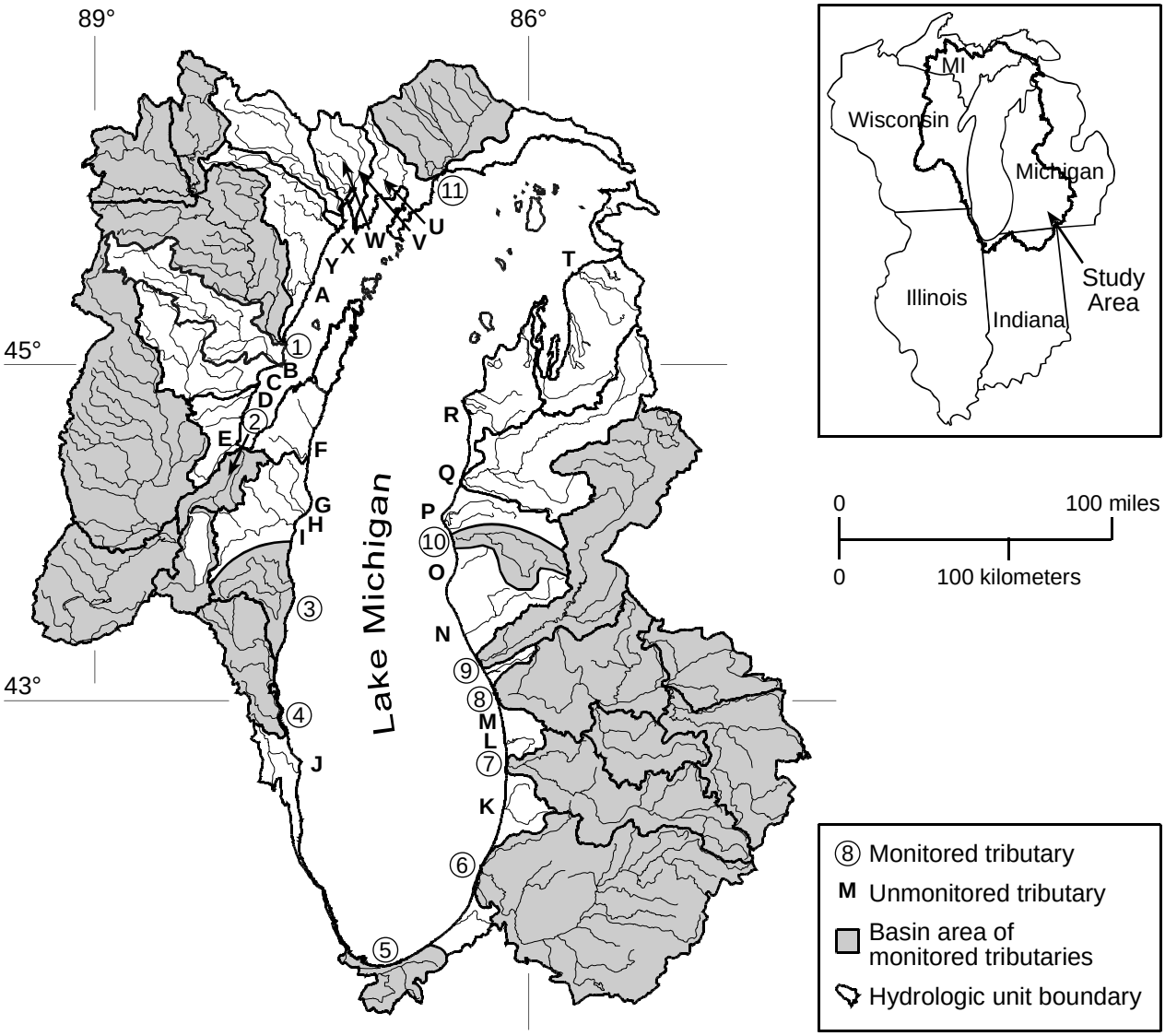


Figure 1. Lake Michigan tributaries.

the Menominee, Fox, Sheboygan, and Milwaukee Rivers in Wisconsin; the Grand Calumet River in Indiana; and the St. Joseph, Kalamazoo, Grand, Muskegon, Pere Marquette, and Manistique Rivers in Michigan.

Discharge was monitored at each tributary, and a total of 405 samples were collected from the eleven sites for water-quality analysis. Hall *et al*. (1998) have published ancillary data collected during sampling including pH, dissolved oxygen, conductance, and temperature. The remainder of this QSIP will describe methods for computing contaminant loads for both monitored and unmonitored tributaries to Lake Michigan

Tributary Load Computation Objectives

Specific contaminant loading objectives of this project are as follows:

1. Compute loads of point and non-point source constituents from 11 monitored tributaries to Lake Michigan including:

Table 1. Identifier Numbers, Station Names, and Station Numbers of Monitored Tributaries to Lake Michigan.

Identifier Number (From Figure 1)	USGS Station Number	USGS Station Name
1	04067651	Menominee River, at mouth, at Marinette, WI
2	040851385	Fox River, Oil Tank Depot at Green Bay, WI
3	040860041	Sheboygan River, at mouth, at Sheboygan, WI
4	04087170	Milwaukee River, at mouth, at Milwaukee, WI
5	04092750	Grand Calumet River, at Indiana Harbor, IN
6	04102533	St. Joseph River at St. Joseph, MI
7	04108660	Kalamazoo River at New Richmond, MI
8	04120250	Grand River at Grand Haven, MI
9	04122150	Muskegon River at Muskegon, MI
10	04122500	Pere Marquette River at Scottville, MI
11	04057005	Manistique River at Manistique, MI

- atrazine and degradates deisopropylatrazine and deethylatrazine,
- filtered and unfiltered mercury,
- nutrients, including total phosphorus, dissolved phosphorus, total nitrogen, Kjeldahl nitrogen, ammonia, dissolved nitrate plus nitrite, and silica,
- other parameters including total solids, particulate organic carbon, dissolved organic carbon, chloride, calcium, magnesium, conductivity, alkalinity, and hardness,
- total PCBs and 34 selected PCB congeners,
- *trans*-nonachlor.

2. Estimate loads of predominately non-point source contaminants from selected unmonitored tributaries to Lake Michigan, including:
   - atrazine and degradates deisopropylatrazine and deethylatrazine,
   - filtered and unfiltered mercury,
   - nutrients, including total phosphorus, dissolved phosphorus, total nitrogen, Kjeldahl nitrogen, ammonia, dissolved nitrate plus nitrite, and silica,
   - *trans*-nonachlor,
   - other parameters, including total solids, particulate organic carbon, dissolved organic carbon, chloride, calcium, magnesium, conductivity, alkalinity, and hardness.
3. Estimate loads of predominately point-source PCBs and PCB congeners from selected unmonitored tributaries to Lake Michigan, including
   - total PCBs and 34 selected PCB congeners.

Personnel Descriptions

David Hall - David Hall is a Hydrologist with the USGS, Water Resources Division, in Middleton, Wisconsin. He earned a BA in Geology from Humboldt State University in 1985, Master of Environmental Pollution Control degree from Penn State University, Capitol Campus, in 1994, and completed additional coursework in water chemistry and hydrogeology at University of Wisconsin-Madison, 1994-96. His research experience includes

modeling of the partitioning, transport, and fate of organic chemicals in the environment, evaluation of agricultural best-management practices, characterizations of nonpoint-source water and air pollution at field-site and regional scales, and statistical analyses of water quality.

Dale Robertson - Dr. Robertson is currently a Research Hydrologist with the USGS, Water Resources Division, in Middleton, Wisconsin. His research interests include developing regional load estimates, determining how different sampling strategies effect load estimates, and examining the influence of environmental factors, watershed management strategies, and in-lake management alternatives on the water quality of rivers and lakes. He has recently completed a project with USEPA to estimate high-flow and long-term average annual nutrient and sediment loading to Lake Michigan and Lake Superior. He is currently working on a project, funded by the National Water Quality Assessment (NAWQA) program of the USGS and the WDNR to determine how different sampling strategies affect load estimates in small streams. He is also working with the WDNR and the University of Wisconsin to estimate regional loading of trace metals to Lake Michigan and determine the allocation of this load to urban and watershed sources.

Method Description

Researcher Responsibilities

David Hall is responsible for all project loading activities, computation of contaminant loads, compilation and reporting of load data, maintenance of the loading data database, and publication of project reports.

Dr. Dale Robertson will act as a consultant in all project tasks, and will specifically provide guidance on the application of methods used to extrapolate loads from the 11 monitored tributaries to unmonitored portions of the basin.

Methods of Load Computation

Task 1: Compute loads of point and non-point source contaminants from 11 monitored tributaries to Lake Michigan, including:

- atrazine and degradates deisopropylatrazine and deethylatrazine,
- filtered and unfiltered mercury,
- nutrients, including total phosphorus, total nitrogen, Kjeldahl nitrogen, ammonia, dissolved nitrate plus nitrite and silica,
- other parameters including total solids, particulate organic carbon, dissolved organic carbon, chloride, calcium, magnesium, conductivity, alkalinity, and hardness,
- total PCBs and 34 selected PCB congeners,
- *trans*-nonachlor.

Eleven tributaries in Wisconsin, Michigan, and Indiana were monitored for discharge and water quality from April 1, 1994 through October 31, 1995. Daily loads of contaminants discharged from each tributary during this 19-month period are to be estimated using the Beale Ratio Estimator method, which produces error estimates associated with loads. Additionally, loads for a 24-month period from January 1, 1994 through December 31, 1995 will be estimated for input to the LMMBP model by an innovative combination of the Beale model output with output from the USGS Estimator Regression Model.

LMTMP Project Results

The Lake Michigan Tributary Monitoring Project results will consist of Beale-model daily contaminant loads and associated error for the 19-month monitored period from April 1, 1994 through October 31, 1995. In summary, Beale model output divides each year of discharge and concentration data into a variable number of strata of averaged daily loads (same average load for each day within the stratum). The total number of strata is determined by an algorithm that minimizes the error associated with the total annual load.

As an extension of the Beale approach, average daily values within each stratum may be converted to discrete daily values (i.e., a different load for each day) by multiplying the average daily load for each stratum by the ratio of discharge on each day divided by the average discharge for the stratum (R. Peter Richards, Heidelberg College, oral communication, June 1998). Thus, days with greater discharge within a stratum have a larger daily load,

which is consistent with the Beale model assumption that contaminant flux increases with increased discharge.

Additional Loads Produced as Input to the Lake Michigan Mass Balance Project Model

For the purposes of producing tributary-load input data for the USEPA LMMBP model, data from the 19-month period will be used to provide estimates of daily contaminant loads for two additional periods: January 1, 1994 through March 31, 1994, and November 1, 1995 through December 31, 1995. Data for these additional periods are required to enable comparisons of tributary loading data collected in other facets of the LMMBP including open-lake monitoring, biological monitoring, and atmospheric monitoring that extended for a 24-month period from January 1, 1994 through December 31, 1995 (Douglas Endicott, USEPA, LLRS, oral communication, February 1998).

Because the Beale Ratio Estimator model does not produce a mathematical formula or other means from which to extrapolate the monitoring-period data to unmonitored periods, a procedure was developed to use the Beale-model daily loads and regression-model loads from the monitored period to "adjust" regression-produced daily loads from the unmonitored period (Dave Dolan, IJC, oral communication, June 1998; R. Peter Richards, Heidelberg College, oral communication, June 1998).

An adjustment coefficient will be computed by dividing the sum of Beale-model daily loads for the period April 1, 1994 through October 31, 1995 by the sum of the Estimator Regression Model loads for the same period. The adjustment coefficient will then be multiplied by each daily load produced by the selected regression model for each of the two unmonitored periods to produce "corrected" daily loads. For example, if the Beale model was producing a sum of daily loads greater than the sum of regression model daily loads for the monitored period, the adjustment coefficient would be greater than one, and the adjustment multiplication would linearly increase each regression-daily load in each of the two unmonitored periods.

The final series of daily contaminant loads used as model input will therefore consist of the following series of daily loads:

January 1, 1994 through March 31, 1994: adjusted regression-model daily loads

April 1, 1994 through October 31, 1995: adjusted Beale-model daily loads

November 1, 1995 through December 31, 1995: adjusted regression-model daily loads.

Selection of the Most Appropriate Regression Model

The USGS Estimator regression software enables the user to evaluate different models using various combinations of simple and transformed variables such as flow, time, and constants. For example, a standard set of variables for a regression on a data series that may demonstrate a trend and also possibly display seasonality is log-flow, log-flow squared, decimal time, decimal-time squared, sine, and cosine terms (Timothy Cohn, USGS, Reston, Virginia, written communication, June 1998). In cases where this suggested set of terms produces an unacceptable output, such as a poor r-squared, unacceptable residual distributions, or any negative daily loads, simpler models can be constructed from fewer terms such as log-flow or square-root flow, with or without a constant. For the purposes of this project, the regression model with the largest r-squared value, the most acceptable residual distributions, and the output most similar in magnitude to Beale-model output will be selected.

Task 2: Estimate loads of predominately non-point source constituents from selected unmonitored tributaries to Lake Michigan, including:

- atrazine and degradates deisopropylatrazine and deethylatrazine,
- filtered and unfiltered mercury,
- nutrients, including total phosphorus, dissolved phosphorus, total nitrogen, Kjeldahl nitrogen, ammonia, dissolved nitrate plus nitrite, and silica,
- *trans*-nonachlor,
- other parameters including total solids, particulate organic carbon, dissolved organic carbon, chloride, calcium, magnesium, conductivity, alkalinity, and hardness.

Unit-Area Yields

Unit-area yields of constituents calculated from the 11 monitored tributaries will be extrapolated to 25 additional unmonitored tributaries with basins larger than 325 km-squared (Figure 1, Table 2) in the Lake Michigan basin to obtain an estimate of the total tributary loads input to Lake Michigan. Locations of both the monitored and unmonitored tributaries are illustrated in Figure 1 from Robertson (1997). The unit-area yields from the monitored basin with the most similar environmental factors will be multiplied by the area of the selected unmonitored basin to obtain loads. Distributions of daily loads from the unmonitored areas will be assumed to resemble the daily load distribution from the monitored tributary.

Surficial deposit and land use data will be used to select the most similar monitored basin (Figure 1, Table 1) from which to extrapolate yield data to each unmonitored basin (Figure 1, Table 1). Geographic information system (GIS/ARC/INFO) coverages of surficial deposits and land use that will be used to define basin characteristics for the extrapolation procedure have been published in Robertson (1997). The generalized coverage of surficial deposits in the Lake Michigan basin was obtained from quatenary geologic maps published by Richmond and Fullerton (1983), Farrand and Bell (1982), and Hobbs and Goebel (1982). The land use coverage was digitized from the National Atlas of the United States of America (USGS, 1970).

The combination of the basin areas of the 11 monitored tributaries and the 25 unmonitored tributaries with basin areas greater than 325 km-squared (Table 2) comprise approximately 87 percent of the land area draining into Lake Michigan (Robertson, 1996). Areas of the 25 selected tributaries will be enlarged to encompass smaller basins (less than 325 km-squared) drained by numerous small tributaries where basin boundaries may be poorly defined and land use and physical properties of the basins may be poorly resolved, thereby obtaining representation of the entire unmonitored area of Lake Michigan.

PCB loads will be estimated for each of the 25 unmonitored rivers listed above (Table 1). Where discharge data exist for an unmonitored tributary for the period of interest, the existing record will be used in load computations. Where no discharge data exist, unit-area water yields will be extrapolated from the most similar monitored basin to the unmonitored basins.

Table 2. Unmonitored Tributaries With Basin Areas Greater than 325 km^2 and Location Identifiers Used in Figure 1.

Unmonitored Tributary	Identifiers on Figure 1
Cedar	A
Peshtigo	B
Oconto	C
Pensaukee	D
Duck	E
Kewaunee	F
East Twin	G
West Twin	H
Manitowoc	I
Root	J
Black (SH)	K
Black (HD)	L
Pigeon	M
White	N
Pentwater	O
Big Sable	P
Manistee	Q
Betsie	R
Boardman	S
Jordan	T
Sturgeon	U
Whitefish	V
Rapid	W
Escanaba	X
Ford	Y

Bed sediment concentrations of PCBs in Lake Michigan tributaries were published in Robertson (1997) and were obtained by Robertson from the USEPA (K. Klewin, USEPA, written communication, 1994). Sediments were sampled either at the river mouth or at the harbor at the river mouth. For each river where sediment chemistry data are available, the median PCB concentration of all samples will be used in the load calculations. Sediment PCB data from the eleven monitored sites will be used to develop a regression model relating sediment concentration to water concentrations. This model will be used to translate the existing database of sediment PCB concentrations in the

unmonitored tributaries to water concentrations to enable the estimation of tributary loads.

Where possible, PCB congener distributions from published literature will be used to assist in determining the loads of individual congeners. Where no PCB concentration data exist for an unmonitored tributary, concentrations will be assumed to be at or near zero.

Record Usage and Management

Data Records

All data generated by the USGS will be recorded in electronic format. All databases are backed up either to floppy disks or 8-mm tape, and will be stored at USGS offices in Middleton, Wisconsin.

Records Management System

A master directory, LMMBP, will be created to hold all data. Separate subdirectories will be created for FINAL results. A complete description of the data directory structure will be included in a 'readme' file located in the master directory.

Records Validation

Computer files are manually validated by visually checking approximately 10% of the data records for accuracy, and by inspection of data plots. Additionally, project results will be reviewed by various personnel as necessary prior to, and after, data submission to the USEPA.

Record Identification, Indexing, and Retention

After completion of the project, all electronic data will be archived on tape or on disks. Electronic archived data and printed materials will be retained for five years after the end of the project.

Records Distribution and Storage

Only final data records will be distributed outside the USGS. These records will be prepared and carefully reviewed by David Hall before distribution and reporting. Interim storage of preliminary data records is described above. Data releases to non-USEPA agencies or to the general public will be cleared through Mr. Glenn Warren, USEPA GLNPO prior to release.

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